



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:49 pm BST

PDB ID : 2EIN
Title : Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully oxidized state
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2007-03-13
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

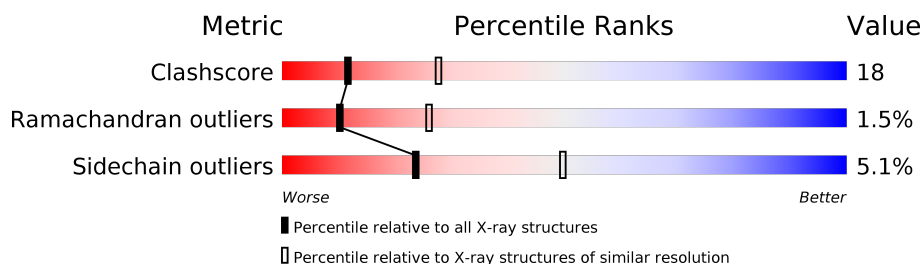
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)


















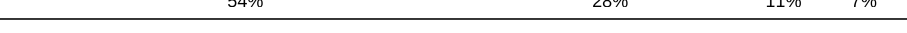
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	

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Mol	Chain	Length	Quality of chain
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
22	PSC	B	230	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 31815 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Cu	0	0
			1	1		
14	N	1	Total	Cu	0	0
			1	1		

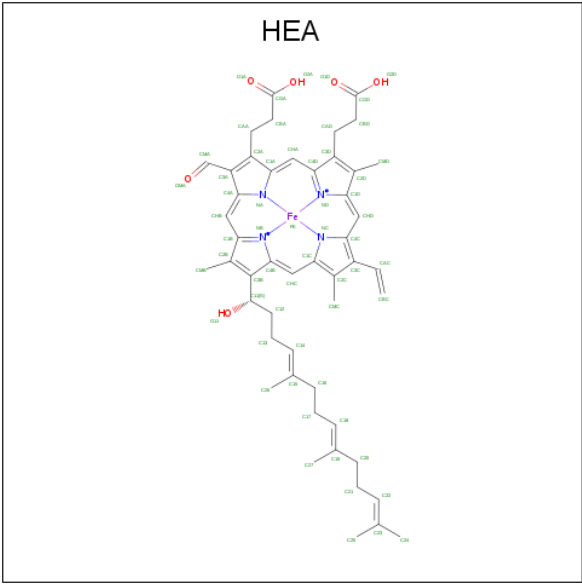
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

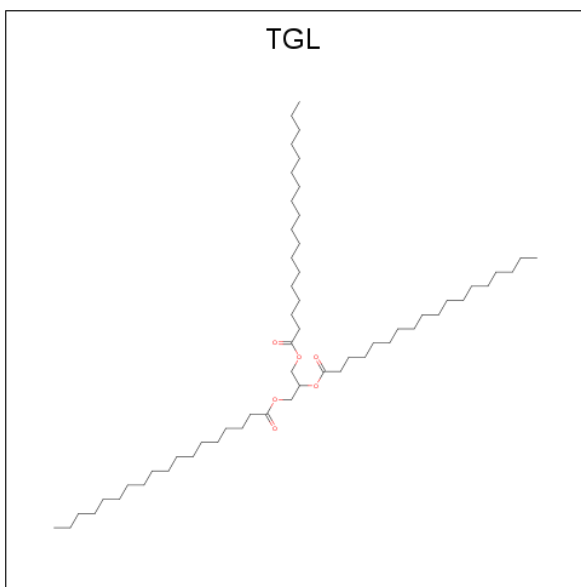
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



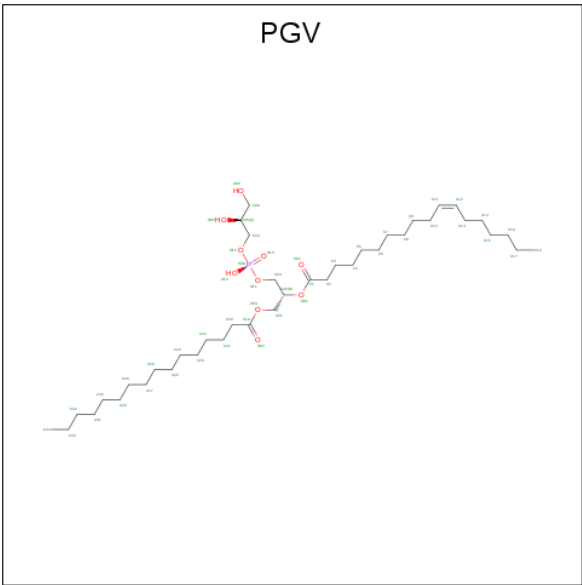
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	A	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	O	1	Total	C	O	0	0
			63	57	6		
18	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

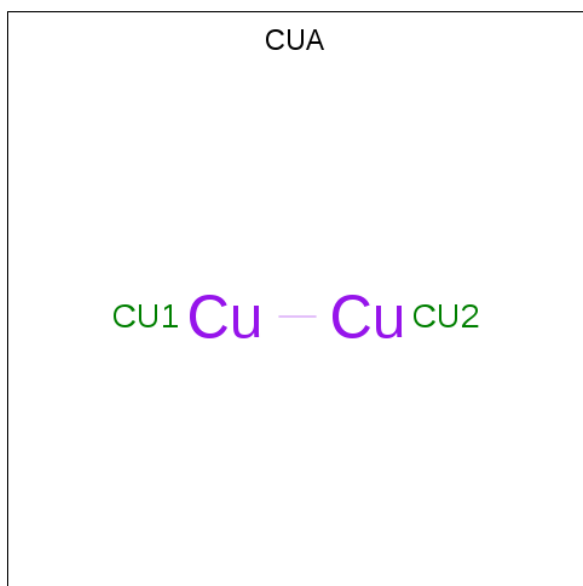
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	P	2	Total	Zn	0	0
			2	2		
20	G	1	Total	Zn	0	0
			1	1		
20	D	1	Total	Zn	0	0
			1	1		
20	B	1	Total	Zn	0	0
			1	1		

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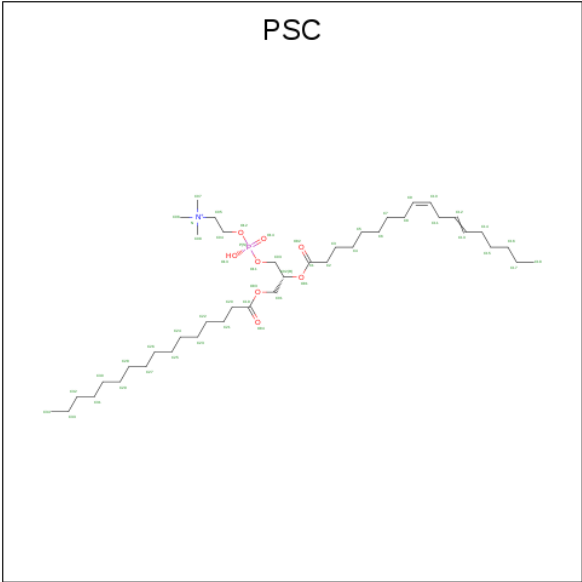
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	1	Total 1	Zn 1	0	0
20	T	1	Total 1	Zn 1	0	0
20	N	2	Total 2	Zn 2	0	0
20	O	1	Total 1	Zn 1	0	0
20	L	1	Total 1	Zn 1	0	0
20	S	1	Total 1	Zn 1	0	0
20	F	2	Total 2	Zn 2	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



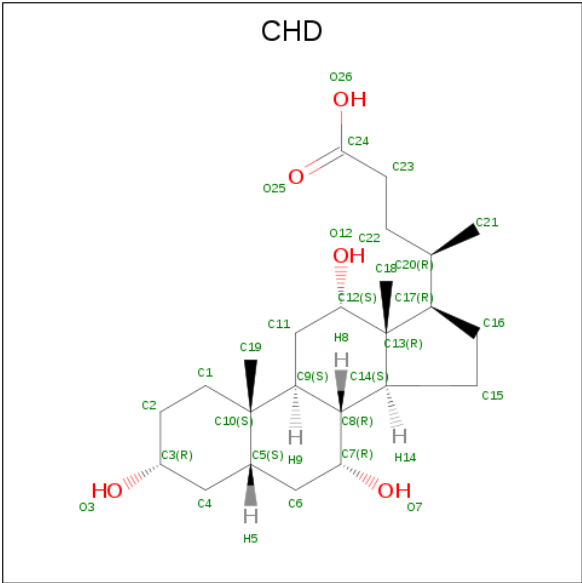
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total 2	Cu 2	0	0
21	O	1	Total 2	Cu 2	0	0

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



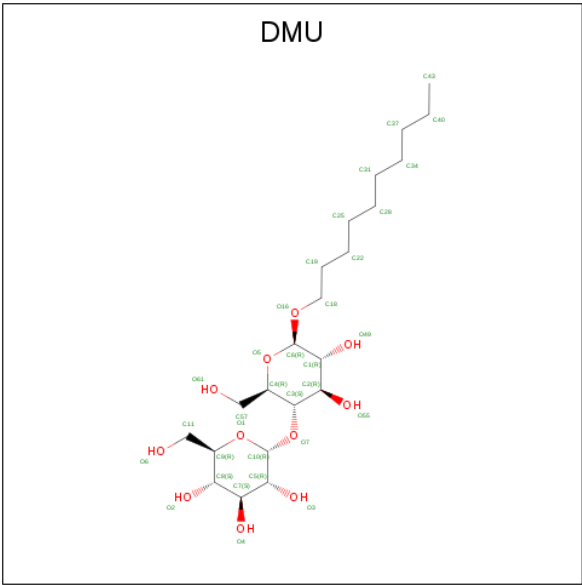
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		
23	G	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0
			29	24	5		

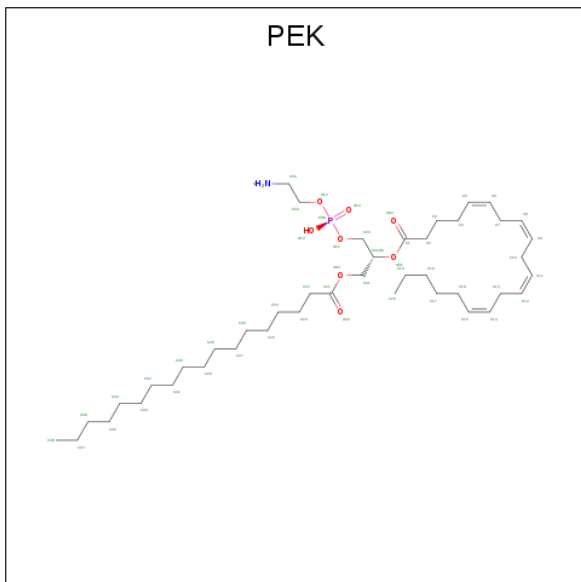
- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

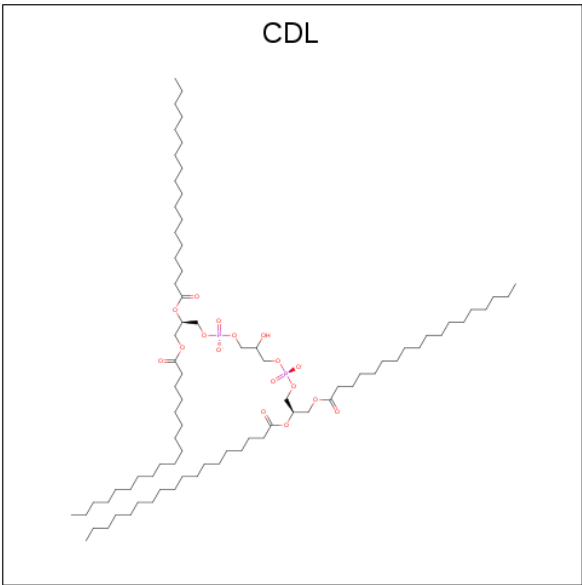
- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(ST

EAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE
(three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	160	Total	O	0	0
			160	160		
27	B	86	Total	O	0	0
			86	86		
27	C	73	Total	O	0	0
			73	73		
27	D	38	Total	O	0	0
			38	38		
27	E	23	Total	O	0	0
			23	23		
27	F	37	Total	O	0	0
			37	37		
27	G	29	Total	O	0	0
			29	29		
27	H	31	Total	O	0	0
			31	31		

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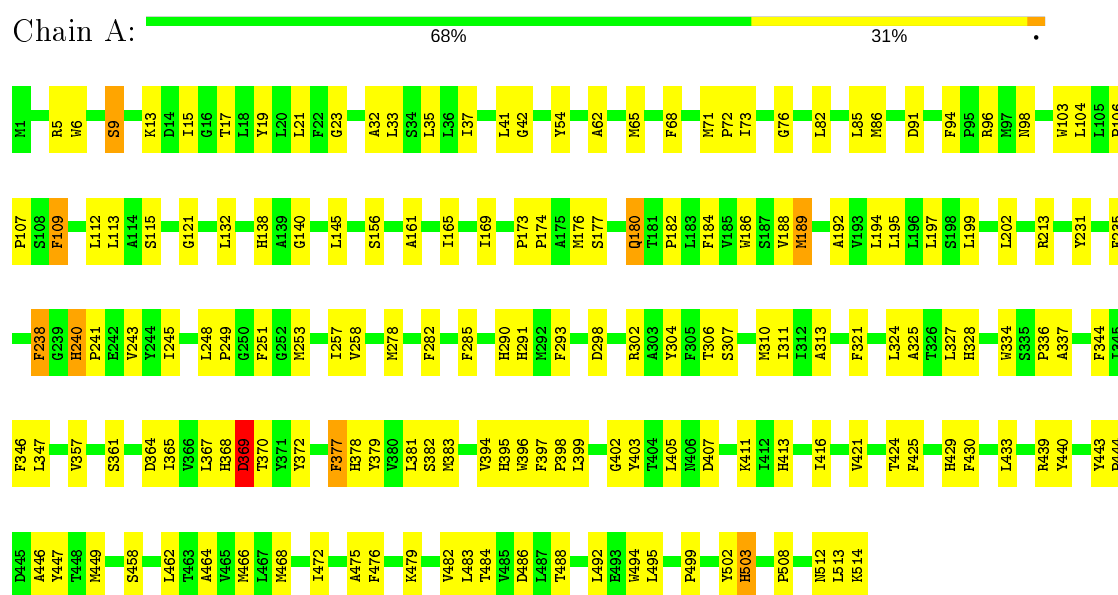
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	I	18	Total 18	O 18	0	0
27	J	9	Total 9	O 9	0	0
27	K	20	Total 20	O 20	0	0
27	L	12	Total 12	O 12	0	0
27	M	11	Total 11	O 11	0	0
27	N	161	Total 161	O 161	0	0
27	O	77	Total 77	O 77	0	0
27	P	72	Total 72	O 72	0	0
27	Q	42	Total 42	O 42	0	0
27	R	22	Total 22	O 22	0	0
27	S	39	Total 39	O 39	0	0
27	T	26	Total 26	O 26	0	0
27	U	28	Total 28	O 28	0	0
27	V	17	Total 17	O 17	0	0
27	W	13	Total 13	O 13	0	0
27	X	13	Total 13	O 13	0	0
27	Y	11	Total 11	O 11	0	0
27	Z	5	Total 5	O 5	0	0

3 Residue-property plots

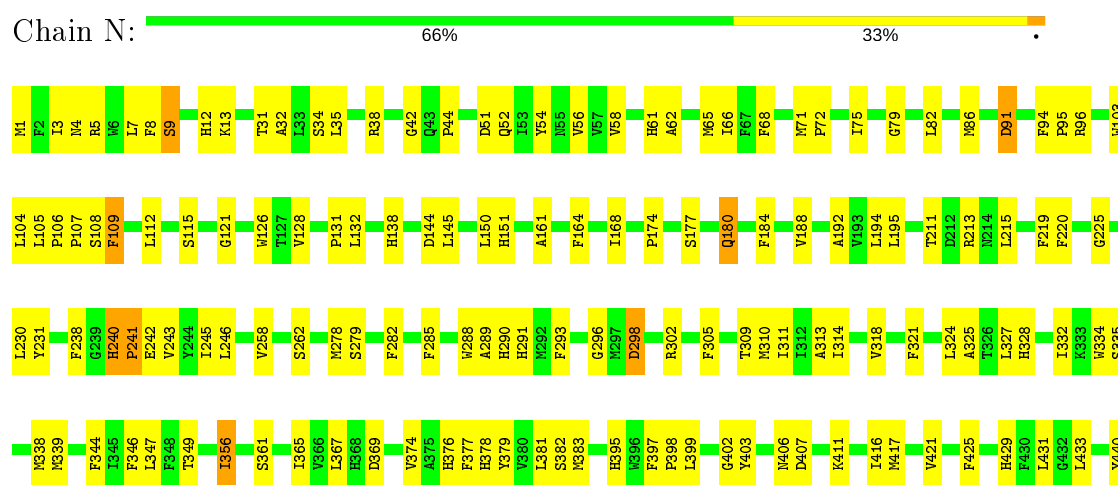
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

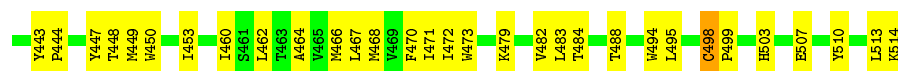
Note EDS was not executed.

• Molecule 1: Cytochrome c oxidase subunit 1

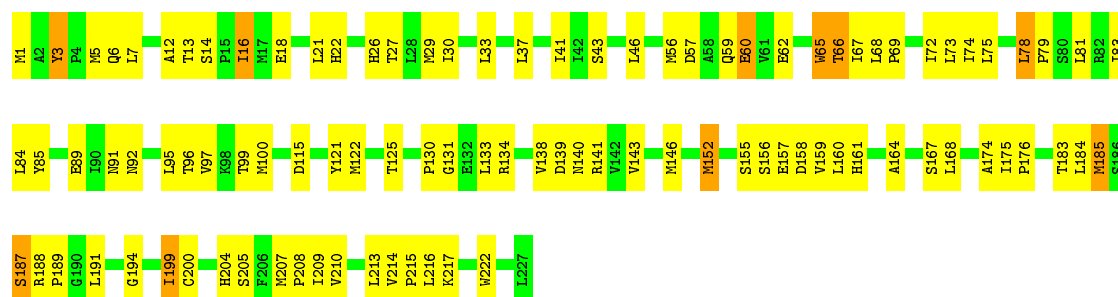


• Molecule 1: Cytochrome c oxidase subunit 1

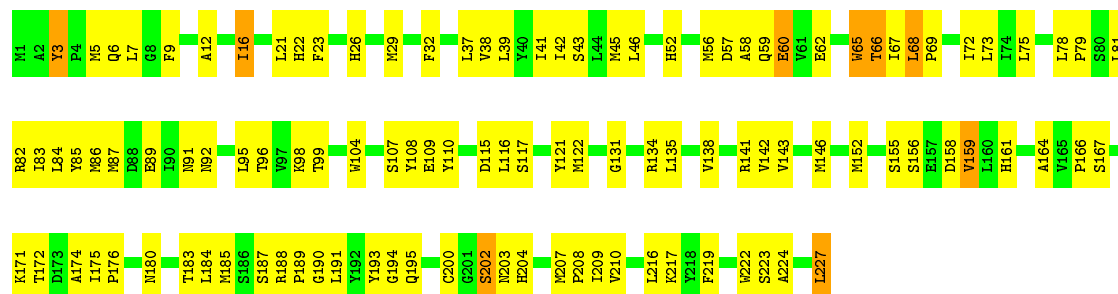




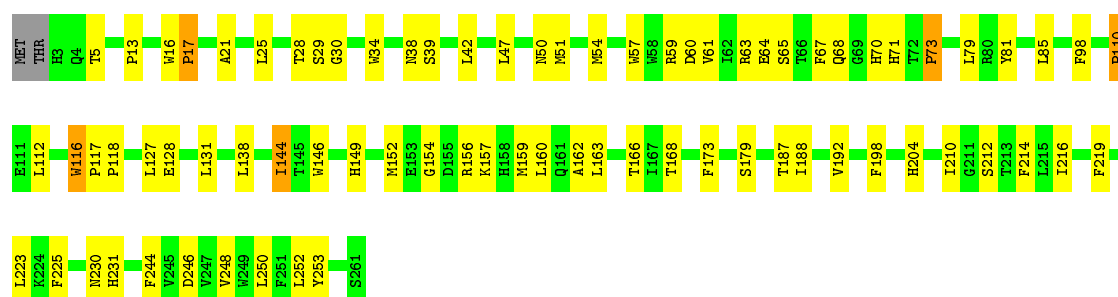
- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3



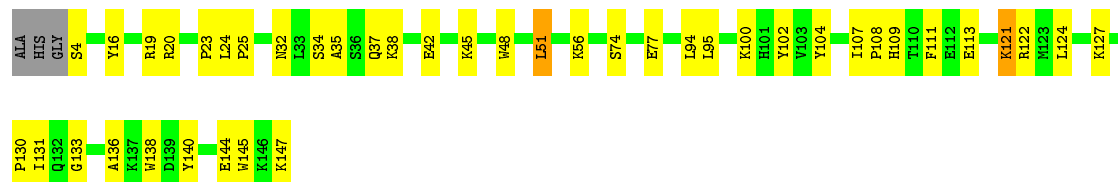
- Molecule 3: Cytochrome c oxidase subunit 3





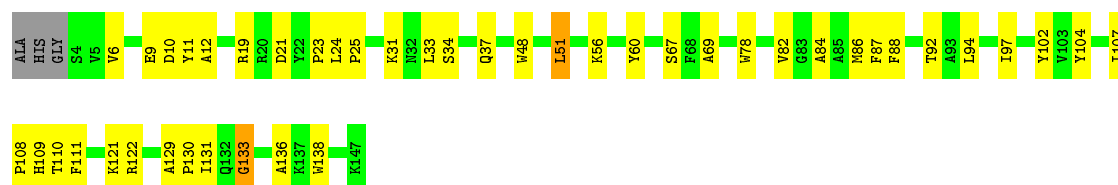
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 69% 27% ..



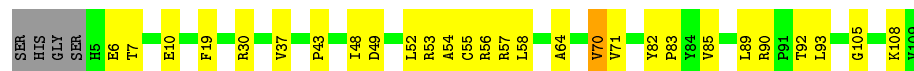
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 68% 29% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E: 71% 25% . .



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R: 68% 27% . .

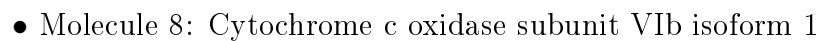
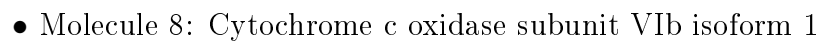
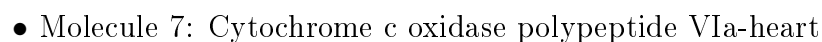
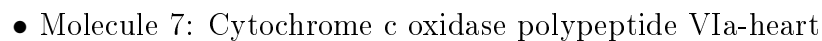


- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F: 68% 28% .



- Molecule 6: Cytochrome c oxidase polypeptide Vb



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  73% 24% ..



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  75% 22% ..



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  70% 16% • 13%



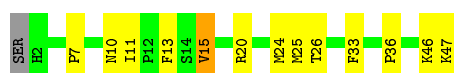
- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  66% 20% • 13%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  70% 26% ..



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  66% 30% ..



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  54% 28% 11% 7%



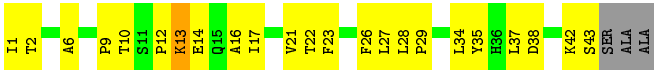
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:

43%

48%

• 7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.81Å 203.58Å 177.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.208 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31815	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.69	0/4156	0.79	0/5678
1	N	0.58	0/4156	0.73	0/5678
2	B	0.68	0/1860	0.87	0/2534
2	O	0.66	0/1860	0.84	1/2534 (0.0%)
3	C	0.69	1/2197 (0.0%)	0.69	0/3005
3	P	0.62	0/2197	0.69	0/3005
4	D	0.63	0/1229	0.74	1/1658 (0.1%)
4	Q	0.66	0/1229	0.71	1/1658 (0.1%)
5	E	0.62	0/871	0.71	0/1182
5	R	0.52	0/871	0.68	0/1182
6	F	0.70	0/765	0.94	3/1038 (0.3%)
6	S	0.67	0/765	0.89	3/1038 (0.3%)
7	G	0.67	1/690 (0.1%)	0.80	1/937 (0.1%)
7	T	0.71	0/690	0.78	1/937 (0.1%)
8	H	0.65	0/682	0.72	0/921
8	U	0.62	0/682	0.74	0/921
9	I	0.69	0/605	0.69	0/802
9	V	0.63	0/605	0.64	0/802
10	J	0.60	0/471	0.71	0/636
10	W	0.62	0/471	0.74	0/636
11	K	0.63	0/398	0.75	0/546
11	X	0.61	0/398	0.76	0/546
12	L	0.80	0/393	0.72	0/526
12	Y	0.64	0/393	0.68	0/526
13	M	0.64	0/345	0.76	0/470
13	Z	0.60	0/345	0.76	0/470
All	All	0.65	2/29324 (0.0%)	0.76	11/39866 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	N	0	1
2	B	0	1
2	O	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	116	TRP	CB-CG	5.36	1.59	1.50
7	G	36	TRP	CB-CG	5.02	1.59	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.42	128.32	111.00
6	S	9	ASP	CB-CG-OD2	6.35	124.02	118.30
6	F	94	HIS	N-CA-C	6.19	127.72	111.00
6	F	9	ASP	CB-CG-OD2	6.15	123.84	118.30
7	G	6	GLY	N-CA-C	5.79	127.59	113.10
2	O	227	LEU	CA-CB-CG	5.63	128.25	115.30
4	D	133	GLY	N-CA-C	5.46	126.74	113.10
4	Q	133	GLY	N-CA-C	5.38	126.55	113.10
6	F	93	PRO	N-CA-C	5.25	125.75	112.10
6	S	93	PRO	N-CA-C	5.22	125.67	112.10
7	T	6	GLY	N-CA-C	5.12	125.90	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	372	TYR	Sidechain
1	A	502	TYR	Sidechain
2	B	85	TYR	Sidechain
1	N	240	HIS	Sidechain
2	O	85	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	162	0
1	N	4027	0	4001	165	0
2	B	1824	0	1833	91	0
2	O	1824	0	1833	101	0
3	C	2110	0	2027	79	0
3	P	2110	0	2027	83	0
4	D	1195	0	1183	38	0
4	Q	1195	0	1183	39	0
5	E	852	0	845	16	0
5	R	852	0	845	22	0
6	F	748	0	728	18	0
6	S	748	0	728	26	0
7	G	675	0	643	38	0
7	T	675	0	643	46	0
8	H	662	0	623	18	0
8	U	662	0	623	15	0
9	I	601	0	613	15	0
9	V	601	0	613	20	0
10	J	460	0	459	11	0
10	W	460	0	459	11	0
11	K	384	0	366	11	0
11	X	384	0	366	13	0
12	L	380	0	380	17	0
12	Y	380	0	380	17	0
13	M	335	0	352	17	0
13	Z	335	0	352	12	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	15	0
17	N	120	0	108	18	0
18	A	126	0	220	11	0
18	L	63	0	110	20	0
18	N	63	0	110	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	O	63	0	110	8	0
18	Y	63	0	110	16	0
19	A	102	0	152	9	0
19	C	102	0	152	7	0
19	N	102	0	152	9	0
19	P	102	0	152	11	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	2	0	0	0	0
20	G	1	0	0	0	0
20	L	1	0	0	0	0
20	N	2	0	0	0	0
20	O	1	0	0	0	0
20	P	2	0	0	0	0
20	S	1	0	0	0	0
20	T	1	0	0	0	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	21	0
22	O	52	0	80	20	0
23	B	29	0	39	5	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	39	4	0
23	P	58	0	78	6	0
23	W	29	0	39	3	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	38	4	0
24	Z	33	0	38	0	0
25	C	106	0	154	20	0
25	G	53	0	77	10	0
25	P	53	0	77	10	0
25	T	106	0	154	23	0
26	C	100	0	156	17	0
26	G	100	0	156	23	0
26	P	100	0	156	17	0
26	T	100	0	156	32	0
27	A	160	0	0	8	0
27	B	86	0	0	3	0
27	C	73	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	D	38	0	0	3	0
27	E	23	0	0	2	0
27	F	37	0	0	1	0
27	G	29	0	0	5	0
27	H	31	0	0	2	0
27	I	18	0	0	1	0
27	J	9	0	0	0	0
27	K	20	0	0	0	0
27	L	12	0	0	0	0
27	M	11	0	0	1	0
27	N	161	0	0	9	0
27	O	77	0	0	5	0
27	P	72	0	0	7	0
27	Q	42	0	0	2	0
27	R	22	0	0	1	0
27	S	39	0	0	1	0
27	T	26	0	0	3	0
27	U	28	0	0	1	0
27	V	17	0	0	3	0
27	W	13	0	0	1	0
27	X	13	0	0	1	0
27	Y	11	0	0	2	0
27	Z	5	0	0	1	0
All	All	31815	0	31298	1087	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1087) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.12	1.11
25:C:264:PEK:H161	25:C:264:PEK:H102	1.38	1.04
7:T:31:CYS:SG	26:T:1269:CDL:H532	1.98	1.04
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.08	1.01
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.45	0.99
22:B:230:PSC:H142	22:B:230:PSC:H343	1.43	0.97
26:G:269:CDL:H541	26:G:269:CDL:H231	1.46	0.97
25:T:1264:PEK:H161	25:T:1264:PEK:H102	1.48	0.96
26:T:1269:CDL:H231	26:T:1269:CDL:H541	1.47	0.95
7:G:84:LYS:HD2	7:G:84:LYS:H	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:1521:TGL:H102	18:O:1521:TGL:H281	1.50	0.94
1:A:503:HIS:CD2	1:A:503:HIS:H	1.82	0.92
12:L:20:ARG:HH12	18:L:522:TGL:HC61	1.34	0.91
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.52	0.90
26:C:270:CDL:H642	26:C:270:CDL:H191	1.54	0.89
12:Y:13:PHE:HA	18:Y:1522:TGL:HC31	1.54	0.89
18:A:521:TGL:H102	18:A:521:TGL:H281	1.51	0.89
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.53	0.89
18:L:522:TGL:HC62	18:L:522:TGL:HC22	1.56	0.87
1:A:278:MET:SD	7:T:5:LYS:HB3	2.15	0.87
26:G:269:CDL:H522	26:G:269:CDL:H202	1.57	0.86
3:C:187:THR:HB	7:G:68:THR:HG21	1.59	0.85
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.59	0.84
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.57	0.84
18:O:1521:TGL:H102	18:O:1521:TGL:C28	2.06	0.84
18:A:521:TGL:H102	18:A:521:TGL:C28	2.07	0.84
18:Y:1522:TGL:HC22	18:Y:1522:TGL:HC62	1.60	0.83
7:G:5:LYS:HB3	1:N:278:MET:SD	2.20	0.82
7:T:84:LYS:HD2	7:T:84:LYS:H	1.42	0.82
1:A:42:GLY:HA3	4:D:104:TYR:OH	1.78	0.82
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.15	0.82
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.44	0.82
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.60	0.82
1:N:488:THR:HB	1:N:495:LEU:HD13	1.62	0.81
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.60	0.80
1:N:42:GLY:HA3	4:Q:104:TYR:OH	1.82	0.79
2:O:57:ASP:H	22:O:1230:PSC:H201	1.45	0.79
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.64	0.78
18:A:523:TGL:HG11	18:A:523:TGL:HC21	1.66	0.78
3:C:54:MET:HE3	26:C:270:CDL:H612	1.64	0.78
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.66	0.77
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.67	0.77
1:A:472:ILE:HD13	18:L:522:TGL:HA91	1.65	0.77
26:G:269:CDL:H541	26:G:269:CDL:C23	2.15	0.77
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.66	0.77
1:N:177:SER:H	1:N:180:GLN:HE21	1.34	0.76
1:A:381:LEU:HB3	17:A:515:HEA:HBC1	1.66	0.76
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.15	0.76
1:N:472:ILE:HG21	18:Y:1522:TGL:CA9	2.16	0.75
7:T:34:ASN:HD22	26:T:1269:CDL:H151	1.52	0.75
18:N:1523:TGL:HC21	18:N:1523:TGL:HG11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.84	0.75
1:N:82:LEU:O	1:N:86:MET:HG3	1.86	0.75
3:C:63:ARG:NE	26:C:270:CDL:HA22	1.97	0.74
4:Q:24:LEU:HD12	5:R:30:ARG:HA	1.67	0.74
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.52	0.74
3:P:187:THR:HB	7:T:68:THR:HG21	1.69	0.74
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.68	0.73
1:N:472:ILE:HG21	18:Y:1522:TGL:HA92	1.67	0.73
6:F:54:ASN:OD1	6:F:76:LYS:HD2	1.89	0.73
2:O:65:TRP:CZ3	22:O:1230:PSC:H331	2.23	0.73
7:T:27:SER:OG	26:T:1269:CDL:H792	1.89	0.73
18:A:521:TGL:H201	18:A:521:TGL:H241	1.71	0.72
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.52	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.37	0.72
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.54	0.72
7:G:45:PRO:HD2	27:G:2152:HOH:O	1.90	0.72
1:N:334:TRP:CZ3	18:N:1523:TGL:HA51	2.24	0.72
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.72	0.71
17:N:516:HEA:H241	2:O:72:ILE:CG2	2.21	0.71
3:P:62:ILE:HD11	3:P:221:ARG:HD2	1.72	0.71
6:S:75:HIS:H	6:S:80:GLN:HE22	1.38	0.71
3:P:213:THR:HG21	19:P:1267:PGV:H11	1.72	0.71
2:O:22:HIS:CE1	2:O:26:HIS:HE1	2.09	0.71
27:Y:4268:HOH:O	13:Z:22:THR:HA	1.91	0.71
4:D:127:LYS:O	4:D:130:PRO:HD3	1.91	0.71
7:G:7:ASP:HB2	27:N:4030:HOH:O	1.90	0.70
1:N:195:LEU:HG	1:N:245:ILE:HD13	1.72	0.70
18:Y:1522:TGL:H242	18:Y:1522:TGL:H202	1.73	0.70
2:O:224:ALA:O	2:O:227:LEU:HG	1.91	0.70
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.22	0.70
3:C:54:MET:HE3	26:C:270:CDL:C61	2.22	0.70
2:O:22:HIS:NE2	2:O:26:HIS:CE1	2.60	0.70
2:B:22:HIS:CE1	2:B:26:HIS:HE1	2.10	0.70
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.73	0.70
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.27	0.70
2:B:156:SER:HB3	2:B:176:PRO:HD3	1.72	0.70
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.73	0.69
12:L:20:ARG:NH1	18:L:522:TGL:HC61	2.07	0.69
1:N:298:ASP:HB3	27:N:3389:HOH:O	1.91	0.69
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.57	0.69
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:SER:N	4:Q:37:GLN:HE21	1.88	0.69
22:B:230:PSC:H222	22:B:230:PSC:H21	1.74	0.69
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.74	0.69
6:S:51:SER:HB2	6:S:91:LEU:HD11	1.74	0.69
2:B:56:MET:HG2	22:B:230:PSC:H211	1.75	0.69
1:N:402:GLY:O	1:N:482:VAL:HG23	1.93	0.69
8:U:7:LYS:O	8:U:8:ILE:HG22	1.94	0.68
1:N:177:SER:H	1:N:180:GLN:NE2	1.91	0.68
3:P:59:ARG:O	3:P:63:ARG:HG3	1.93	0.68
2:B:143:VAL:HB	2:B:222:TRP:CE3	2.29	0.68
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.27	0.68
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.29	0.68
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.75	0.68
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.76	0.68
18:L:522:TGL:H242	18:L:522:TGL:H202	1.75	0.68
1:A:65:MET:HE3	17:A:515:HEA:HMC3	1.76	0.68
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.06	0.68
3:C:187:THR:CB	7:G:68:THR:HG21	2.25	0.67
27:A:4207:HOH:O	7:T:9:GLY:HA3	1.94	0.67
1:A:365:ILE:HD11	27:A:4150:HOH:O	1.94	0.67
26:G:269:CDL:H511	26:G:269:CDL:H172	1.77	0.67
1:N:381:LEU:HB3	17:N:515:HEA:HBC1	1.76	0.67
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.77	0.67
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.76	0.67
2:B:22:HIS:NE2	2:B:26:HIS:CE1	2.63	0.66
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.78	0.66
2:B:68:LEU:O	2:B:72:ILE:HD12	1.95	0.66
7:T:30:LEU:HD12	26:T:1269:CDL:H252	1.77	0.66
7:G:31:CYS:SG	26:G:269:CDL:H532	2.36	0.66
1:N:503:HIS:HB2	27:Y:3093:HOH:O	1.94	0.66
2:O:56:MET:HA	22:O:1230:PSC:C20	2.26	0.66
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.31	0.66
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.30	0.66
26:P:1270:CDL:H431	27:W:4131:HOH:O	1.95	0.66
6:S:94:HIS:CD2	6:S:95:GLN:H	2.14	0.66
1:N:479:LYS:HD3	27:N:4148:HOH:O	1.96	0.65
7:T:70:PHE:HB2	25:T:1264:PEK:H041	1.78	0.65
2:O:7:LEU:HD11	18:O:1521:TGL:H161	1.78	0.65
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	1.79	0.65
18:O:1521:TGL:H201	18:O:1521:TGL:H241	1.78	0.65
6:F:92:VAL:HG23	6:F:92:VAL:O	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:TYR:O	1:N:383:MET:HB2	1.95	0.65
2:B:22:HIS:CE1	2:B:26:HIS:CE1	2.84	0.65
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.01	0.65
1:A:165:ILE:O	1:A:169:ILE:HG12	1.97	0.65
1:N:240:HIS:O	1:N:243:VAL:HG22	1.97	0.65
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.79	0.65
18:A:521:TGL:H161	2:B:7:LEU:HD11	1.79	0.64
25:C:264:PEK:C16	25:C:264:PEK:H102	2.21	0.64
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.79	0.64
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.12	0.64
3:C:210:ILE:HG23	19:C:267:PGV:H102	1.77	0.64
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.79	0.64
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.09	0.64
2:O:209:ILE:HA	27:O:3158:HOH:O	1.98	0.64
1:A:377:PHE:CE2	1:A:378:HIS:CE1	2.86	0.64
1:A:382:SER:HA	17:A:515:HEA:HMC2	1.79	0.64
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.32	0.64
1:A:298:ASP:HB3	27:A:2389:HOH:O	1.98	0.64
2:O:57:ASP:N	22:O:1230:PSC:H201	2.11	0.64
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.63	0.64
3:C:246:ASP:HB2	27:C:4064:HOH:O	1.97	0.64
10:W:45:TYR:O	10:W:48:TYR:HB3	1.98	0.64
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.79	0.63
19:C:267:PGV:H182	26:C:270:CDL:H673	1.80	0.63
1:A:488:THR:HB	1:A:495:LEU:HD13	1.81	0.63
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.80	0.63
7:T:34:ASN:ND2	26:T:1269:CDL:H151	2.12	0.63
11:X:24:PHE:O	11:X:28:VAL:HG12	1.99	0.63
7:G:4:ALA:CB	1:N:282:PHE:HA	2.29	0.63
2:O:22:HIS:CE1	2:O:26:HIS:CE1	2.86	0.63
11:X:54:ARG:HG3	11:X:54:ARG:HH21	1.62	0.63
6:S:94:HIS:CG	6:S:95:GLN:H	2.17	0.63
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.81	0.63
1:A:466:MET:HG2	13:M:26:PHE:CD2	2.34	0.63
19:C:267:PGV:H172	26:C:270:CDL:H662	1.81	0.62
26:P:1270:CDL:H112	27:P:4194:HOH:O	1.98	0.62
1:A:347:LEU:HD13	1:A:383:MET:SD	2.38	0.62
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.35	0.62
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.34	0.62
1:A:407:ASP:O	1:A:411:LYS:HG3	2.00	0.62
1:N:324:LEU:HD13	2:O:41:ILE:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:161:HIS:CE1	2:O:200:CYS:SG	2.92	0.62
2:B:1:FME:SD	2:B:133:LEU:HD11	2.40	0.62
1:N:347:LEU:HD13	1:N:383:MET:SD	2.39	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.39	0.62
27:P:4092:HOH:O	6:S:1:ALA:HB2	2.00	0.62
2:O:42:ILE:O	2:O:46:LEU:HG	2.00	0.61
2:O:82:ARG:HG2	2:O:86:MET:HE1	1.82	0.61
1:A:413:HIS:NE2	1:A:468:MET:HB2	2.15	0.61
2:B:62:GLU:O	2:B:66:THR:HB	2.00	0.61
5:R:31:LYS:HE2	5:R:35:THR:OG1	2.00	0.61
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	1.81	0.61
1:N:416:ILE:HG22	1:N:464:ALA:HB2	1.82	0.61
3:P:112:LEU:HB3	3:P:118:PRO:HB3	1.82	0.61
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.82	0.61
10:W:30:ILE:O	10:W:34:VAL:HG23	2.00	0.61
1:A:367:LEU:HD21	1:A:433:LEU:HD23	1.82	0.61
1:N:103:TRP:O	3:P:21:ALA:HB1	2.01	0.61
3:P:47:LEU:O	3:P:51:MET:HG2	2.01	0.61
3:C:204:HIS:HD2	3:C:248:VAL:HG12	1.65	0.61
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.65	0.61
19:N:1524:PGV:H062	27:Z:3160:HOH:O	2.01	0.61
3:C:212:SER:O	3:C:216:ILE:HG13	2.01	0.60
1:A:112:LEU:HG	27:A:2073:HOH:O	2.00	0.60
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.83	0.60
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.82	0.60
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.36	0.60
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.82	0.60
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.82	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.49	0.60
19:A:524:PGV:H062	27:M:2160:HOH:O	2.01	0.60
1:N:128:VAL:HG12	1:N:128:VAL:O	2.02	0.60
8:H:60:TYR:C	8:H:60:TYR:CD1	2.75	0.60
3:P:157:LYS:HE2	27:P:3156:HOH:O	2.01	0.60
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.37	0.60
1:N:54:TYR:HB2	27:N:3113:HOH:O	2.02	0.60
3:C:168:THR:HG22	25:C:265:PEK:H14	1.84	0.59
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.84	0.59
6:F:85:CYS:SG	6:F:87:THR:HG23	2.42	0.59
3:C:204:HIS:HD2	3:C:248:VAL:CG1	2.16	0.59
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.83	0.59
7:G:17:ARG:HD2	27:G:2309:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:HIS:CD2	10:J:22:LEU:HG	2.37	0.59
10:J:40:LEU:HD12	23:J:60:CHD:H183	1.85	0.59
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.03	0.59
6:S:14:THR:HB	10:W:9:GLN:NE2	2.18	0.59
1:N:406:ASN:ND2	19:N:1524:PGV:H032	2.17	0.59
9:V:65:LYS:O	11:X:54:ARG:NH1	2.36	0.59
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.67	0.59
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.85	0.59
25:C:264:PEK:H041	7:G:70:PHE:HB2	1.85	0.59
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.91	0.58
4:D:102:TYR:HD1	13:M:35:TYR:HE1	1.51	0.58
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.58
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.85	0.58
1:A:240:HIS:O	1:A:243:VAL:HG22	2.03	0.58
2:B:146:MET:HA	2:B:213:LEU:HD12	1.85	0.58
1:N:115:SER:O	1:N:121:GLY:HA2	2.02	0.58
13:Z:17:ILE:O	13:Z:21:VAL:HG23	2.02	0.58
3:C:168:THR:CG2	25:C:265:PEK:H14	2.34	0.58
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.66	0.58
4:D:131:ILE:H	4:D:131:ILE:HD12	1.68	0.58
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.85	0.58
2:B:157:GLU:HA	27:B:4023:HOH:O	2.02	0.58
18:O:1521:TGL:H222	18:O:1521:TGL:HA82	1.85	0.58
1:A:311:ILE:HD12	26:T:1269:CDL:H212	1.86	0.58
1:A:449:MET:SD	2:B:5:MET:HG2	2.44	0.58
3:P:63:ARG:NH1	10:W:20:VAL:O	2.34	0.58
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.86	0.58
18:L:522:TGL:C24	18:L:522:TGL:H202	2.34	0.58
3:P:30:GLY:HA2	3:P:42:LEU:HB3	1.85	0.58
1:A:514:LYS:NZ	27:A:2395:HOH:O	2.37	0.58
25:T:1264:PEK:H71	25:T:1264:PEK:H32	1.85	0.58
1:A:94:PHE:HE1	3:C:79:LEU:HD23	1.69	0.57
1:N:335:SER:O	1:N:339:MET:HG3	2.03	0.57
2:B:66:THR:HG22	2:B:67:ILE:N	2.17	0.57
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.86	0.57
2:B:74:ILE:HD11	26:T:1269:CDL:H452	1.86	0.57
7:T:31:CYS:SG	26:T:1269:CDL:C53	2.86	0.57
1:N:290:HIS:CD2	1:N:291:HIS:NE2	2.73	0.57
3:P:15:PRO:O	3:P:19:THR:HG23	2.04	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.57
2:B:1:FME:SD	2:B:133:LEU:CD1	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:HG22	2:B:27:THR:HG21	1.86	0.57
25:G:1263:PEK:H9	3:P:244:PHE:HA	1.85	0.57
3:P:126:PRO:HG2	3:P:127:LEU:HD22	1.86	0.57
7:T:47:PHE:HE1	7:T:49:PRO:HG3	1.70	0.57
1:A:13:LYS:HE3	1:A:85:LEU:HD21	1.86	0.57
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.40	0.57
1:A:41:LEU:HD11	1:A:54:TYR:OH	2.05	0.57
3:C:204:HIS:CD2	3:C:248:VAL:HG12	2.39	0.57
3:C:51:MET:SD	26:C:270:CDL:H622	2.44	0.57
1:A:405:LEU:HD23	1:A:475:ALA:HB2	1.87	0.57
18:A:521:TGL:HC22	27:I:2383:HOH:O	2.05	0.57
1:N:382:SER:HA	17:N:515:HEA:HMC2	1.86	0.57
1:A:112:LEU:C	1:A:112:LEU:HD23	2.26	0.57
1:A:253:MET:O	1:A:257:ILE:HG13	2.04	0.57
2:B:99:THR:HG22	2:B:152:MET:CE	2.35	0.57
2:B:56:MET:HA	22:B:230:PSC:C20	2.35	0.57
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.39	0.57
2:O:56:MET:HA	22:O:1230:PSC:H202	1.87	0.56
1:A:416:ILE:HG22	1:A:464:ALA:HB2	1.87	0.56
1:A:492:LEU:O	1:A:492:LEU:HD12	2.04	0.56
18:A:521:TGL:HA82	18:A:521:TGL:H222	1.86	0.56
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.05	0.56
1:A:115:SER:O	1:A:121:GLY:HA2	2.06	0.56
3:P:187:THR:CB	7:T:68:THR:HG21	2.34	0.56
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.39	0.56
2:O:82:ARG:HG2	2:O:86:MET:CE	2.36	0.56
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.06	0.56
25:C:265:PEK:H371	26:G:269:CDL:H261	1.87	0.56
25:C:265:PEK:C38	26:G:269:CDL:H273	2.35	0.56
5:R:67:ILE:O	5:R:71:VAL:HG23	2.06	0.56
23:B:1086:CHD:H14	27:B:2112:HOH:O	2.05	0.56
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.87	0.56
6:S:48:LEU:O	6:S:50:PRO:HD3	2.06	0.56
1:A:103:TRP:O	3:C:21:ALA:HB1	2.05	0.56
1:A:484:THR:HB	13:M:2:THR:OG1	2.06	0.56
1:N:31:THR:HG23	17:N:515:HEA:H14	1.87	0.56
1:N:52:GLN:O	1:N:56:VAL:HG23	2.06	0.56
4:Q:69:ALA:O	5:R:109:VAL:HG12	2.05	0.56
19:P:1267:PGV:H161	19:P:1267:PGV:H12	1.87	0.56
6:S:16:LEU:O	6:S:20:VAL:HG23	2.06	0.56
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:O	1:A:107:PRO:HD2	2.06	0.55
4:D:102:TYR:CD1	13:M:35:TYR:HE1	2.24	0.55
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.87	0.55
1:N:310:MET:O	2:O:73:LEU:HD13	2.06	0.55
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.21	0.55
1:A:399:LEU:HB2	1:A:494:TRP:CE3	2.41	0.55
6:F:16:LEU:O	6:F:16:LEU:HD12	2.06	0.55
2:O:23:PHE:CE2	2:O:79:PRO:HG2	2.42	0.55
1:A:381:LEU:HB3	17:A:515:HEA:CBC	2.35	0.55
7:G:2:SER:O	25:G:1263:PEK:H322	2.07	0.55
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.89	0.55
18:Y:1522:TGL:H272	18:Y:1522:TGL:H231	1.87	0.55
2:B:57:ASP:H	22:B:230:PSC:H201	1.71	0.55
1:A:173:PRO:HD2	1:A:176:MET:SD	2.45	0.55
12:Y:40:VAL:O	12:Y:44:LEU:HG	2.07	0.55
3:C:57:TRP:O	3:C:61:VAL:HG23	2.07	0.55
2:O:193:TYR:CD1	2:O:210:VAL:HG22	2.42	0.55
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.87	0.55
1:A:324:LEU:HD13	2:B:41:ILE:HG21	1.89	0.55
1:A:398:PRO:HA	1:A:403:TYR:O	2.07	0.55
1:A:113:LEU:HD12	18:L:522:TGL:H292	1.89	0.55
7:G:66:ASN:HD21	7:G:79:PRO:HD2	1.72	0.55
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.72	0.55
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.88	0.55
3:P:213:THR:CG2	19:P:1267:PGV:H11	2.36	0.55
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.54
1:N:144:ASP:CG	1:N:213:ARG:HH21	2.11	0.54
1:N:184:PHE:O	1:N:188:VAL:HG23	2.07	0.54
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.89	0.54
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.89	0.54
2:B:158:ASP:O	2:B:176:PRO:HG3	2.06	0.54
19:A:524:PGV:H311	13:M:16:ALA:HA	1.89	0.54
1:N:367:LEU:HD21	1:N:433:LEU:HD23	1.89	0.54
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.89	0.54
25:C:265:PEK:H22	27:G:4145:HOH:O	2.07	0.54
7:T:45:PRO:HD2	27:T:3152:HOH:O	2.07	0.54
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.43	0.54
6:F:77:GLY:O	6:F:90:LYS:HE2	2.07	0.54
8:H:46:LYS:NZ	8:U:55:TRP:HB2	2.23	0.54
9:I:23:GLY:O	9:I:27:VAL:HG23	2.08	0.54
18:O:1521:TGL:HC22	27:V:3383:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:39:ASN:O	13:M:43:SER:HB2	2.08	0.54
1:N:324:LEU:HD13	2:O:41:ILE:HG22	1.90	0.54
27:G:4051:HOH:O	2:O:67:ILE:HD11	2.07	0.54
7:T:2:SER:O	25:T:263:PEK:H322	2.07	0.54
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.89	0.54
1:N:104:LEU:O	1:N:107:PRO:HD2	2.08	0.54
1:N:132:LEU:O	1:N:132:LEU:HD12	2.08	0.54
2:O:155:SER:O	2:O:174:ALA:HB1	2.08	0.54
2:B:138:VAL:HG22	2:B:210:VAL:CG2	2.38	0.54
2:B:99:THR:HG22	2:B:152:MET:HE2	1.90	0.54
3:C:68:GLN:HB2	3:C:70:HIS:HD2	1.73	0.54
1:A:5:ARG:O	1:A:9:SER:HB2	2.08	0.54
2:O:216:LEU:O	2:O:219:PHE:HB3	2.08	0.54
1:A:33:LEU:HD23	12:L:36:PRO:HB3	1.89	0.53
1:N:65:MET:HB3	17:N:515:HEA:HAC	1.90	0.53
2:O:121:TYR:O	2:O:138:VAL:HA	2.08	0.53
24:P:1272:DMU:H25	25:T:1264:PEK:H341	1.90	0.53
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.07	0.53
1:A:443:TYR:HD1	1:A:447:TYR:HB2	1.72	0.53
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.43	0.53
18:Y:1522:TGL:C24	18:Y:1522:TGL:H202	2.37	0.53
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.74	0.53
9:V:5:ALA:O	9:V:7:PRO:HD3	2.09	0.53
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.22	0.53
2:B:69:PRO:HG3	22:B:230:PSC:H183	1.91	0.53
4:D:94:LEU:HD23	11:K:28:VAL:HG21	1.89	0.53
4:D:100:LYS:HE2	11:K:37:GLY:O	2.07	0.53
3:P:225:PHE:HA	27:P:3236:HOH:O	2.09	0.53
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.22	0.53
6:S:62:CYS:SG	6:S:84:SER:HB3	2.49	0.53
1:A:86:MET:HB3	1:A:182:PRO:HG2	1.91	0.53
1:A:503:HIS:CD2	1:A:503:HIS:N	2.58	0.53
3:C:98:PHE:CZ	3:C:252:LEU:HD23	2.44	0.53
1:N:399:LEU:HA	1:N:498:CYS:HB3	1.90	0.53
1:N:344:PHE:C	1:N:344:PHE:CD1	2.81	0.53
1:N:35:LEU:HD11	1:N:462:LEU:HD13	1.91	0.53
1:N:466:MET:HG2	13:Z:26:PHE:CD2	2.44	0.53
1:A:306:THR:O	1:A:310:MET:HG3	2.09	0.53
24:C:272:DMU:H25	25:C:264:PEK:H341	1.90	0.53
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.91	0.53
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:PRO:HD2	12:L:7:PRO:HD3	1.91	0.53
4:D:102:TYR:HD1	13:M:35:TYR:CE1	2.26	0.53
3:P:118:PRO:HD2	3:P:121:ILE:HG13	1.91	0.53
18:Y:1522:TGL:H211	18:Y:1522:TGL:HA72	1.91	0.53
6:S:51:SER:CB	6:S:91:LEU:HD11	2.39	0.52
1:N:472:ILE:HD13	18:Y:1522:TGL:HA91	1.91	0.52
2:B:216:LEU:O	2:B:216:LEU:HD12	2.09	0.52
2:O:141:ARG:NH1	2:O:191:LEU:HD11	2.24	0.52
19:C:267:PGV:H161	19:C:267:PGV:H12	1.90	0.52
2:O:68:LEU:HB3	22:O:1230:PSC:H182	1.91	0.52
3:C:29:SER:HB3	3:C:42:LEU:CD1	2.40	0.52
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.44	0.52
1:N:407:ASP:O	1:N:411:LYS:HG3	2.09	0.52
4:Q:97:ILE:HG13	11:X:32:MET:HG3	1.92	0.52
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.92	0.52
2:O:108:TYR:CE1	2:O:142:VAL:HG21	2.45	0.52
26:T:1269:CDL:H342	26:T:1269:CDL:OA7	2.10	0.52
22:B:230:PSC:C07	9:I:10:ARG:NH2	2.73	0.52
7:G:34:ASN:HD22	26:G:269:CDL:H151	1.75	0.52
27:O:4075:HOH:O	4:Q:108:PRO:HG3	2.08	0.52
25:T:1264:PEK:C16	25:T:1264:PEK:H102	2.32	0.52
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.91	0.52
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.45	0.52
26:C:270:CDL:H112	27:C:4234:HOH:O	2.09	0.52
3:C:73:PRO:HB2	27:C:4140:HOH:O	2.10	0.52
9:V:58:LYS:O	9:V:62:GLU:HG3	2.09	0.52
19:A:524:PGV:H301	19:A:524:PGV:H152	1.91	0.52
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.91	0.52
13:M:31:GLY:HA3	24:M:526:DMU:H9	1.91	0.52
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.45	0.52
2:B:209:ILE:HA	27:B:2158:HOH:O	2.09	0.52
1:N:443:TYR:HE1	1:N:448:THR:HA	1.73	0.52
1:A:514:LYS:HE2	27:F:2339:HOH:O	2.10	0.51
23:B:1086:CHD:H20	7:T:18:PHE:HD2	1.75	0.51
2:B:29:MET:HE2	2:B:30:ILE:HG13	1.92	0.51
3:C:127:LEU:HD12	3:C:131:LEU:HD22	1.92	0.51
4:D:107:ILE:CD1	11:K:39:GLU:HB2	2.40	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
3:C:68:GLN:HE21	3:C:70:HIS:CD2	2.29	0.51
2:B:222:TRP:HB2	9:I:71:SER:HB2	1.91	0.51
1:N:243:VAL:HB	17:N:516:HEA:HAC	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:156:ARG:HE	23:P:1271:CHD:H232	1.76	0.51
7:T:6:GLY:O	25:T:263:PEK:H311	2.11	0.51
11:X:19:ALA:HA	27:X:4125:HOH:O	2.10	0.51
12:Y:11:ILE:HG13	12:Y:13:PHE:O	2.10	0.51
3:C:60:ASP:O	3:C:64:GLU:HG3	2.10	0.51
12:L:20:ARG:HH22	18:L:522:TGL:HC32	1.75	0.51
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.93	0.51
2:O:98:LYS:HE3	2:O:109:GLU:HB2	1.92	0.51
27:N:3198:HOH:O	3:P:17:PRO:HG2	2.11	0.51
25:C:265:PEK:H371	26:G:269:CDL:C26	2.41	0.51
1:N:219:PHE:HZ	3:P:199:VAL:HG21	1.76	0.51
1:N:398:PRO:HA	1:N:403:TYR:O	2.10	0.51
6:S:55:LYS:HA	6:S:74:LEU:O	2.11	0.51
6:S:94:HIS:CD2	6:S:95:GLN:N	2.79	0.51
1:N:472:ILE:CG2	18:Y:1522:TGL:HA92	2.36	0.51
3:P:67:PHE:HA	10:W:9:GLN:HG2	1.92	0.51
3:P:80:ARG:HG2	3:P:233:PHE:CE2	2.46	0.51
3:P:198:PHE:CD2	25:T:1264:PEK:H032	2.46	0.51
2:B:141:ARG:HH11	2:B:191:LEU:HD21	1.75	0.51
26:G:269:CDL:C54	26:G:269:CDL:H231	2.29	0.51
9:I:58:LYS:O	9:I:62:GLU:HG3	2.10	0.51
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.93	0.51
18:A:523:TGL:HG11	18:A:523:TGL:CC2	2.39	0.51
3:P:116:TRP:CZ2	3:P:193:TYR:HD1	2.29	0.51
7:T:23:LEU:C	7:T:26:PRO:HD2	2.31	0.51
1:A:37:ILE:HG21	17:A:515:HEA:HMA	1.93	0.51
2:B:164:ALA:O	2:B:194:GLY:HA3	2.10	0.51
19:C:267:PGV:H182	26:C:270:CDL:C67	2.41	0.51
1:A:508:PRO:HD2	3:C:5:THR:OG1	2.10	0.51
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.46	0.51
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.93	0.51
3:P:80:ARG:HG2	3:P:233:PHE:HE2	1.76	0.51
1:A:243:VAL:HB	17:A:516:HEA:HAC	1.93	0.51
2:B:3:TYR:N	2:B:3:TYR:CD2	2.79	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.46	0.51
6:F:55:LYS:HA	6:F:74:LEU:O	2.10	0.51
1:N:1:FME:HCN	1:N:4:ASN:H	1.76	0.51
1:N:349:THR:HG21	2:O:38:VAL:HG21	1.93	0.51
1:N:346:PHE:CE1	2:O:39:LEU:HB2	2.46	0.51
1:A:82:LEU:O	1:A:86:MET:HG3	2.10	0.50
4:D:113:GLU:HG3	27:D:2281:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:LEU:HD22	10:J:50:LEU:O	2.10	0.50
1:A:429:HIS:HB3	18:A:521:TGL:HB41	1.93	0.50
6:F:72:PHE:CE2	6:F:82:CYS:HA	2.47	0.50
26:P:1270:CDL:C19	26:P:1270:CDL:H642	2.34	0.50
1:A:379:TYR:O	1:A:383:MET:HB2	2.11	0.50
1:A:94:PHE:CE1	3:C:79:LEU:HD23	2.46	0.50
23:B:1086:CHD:H162	7:T:18:PHE:CE2	2.46	0.50
1:N:219:PHE:CZ	3:P:199:VAL:HG21	2.47	0.50
1:N:406:ASN:HD21	19:N:1524:PGV:H032	1.75	0.50
1:N:443:TYR:HD1	1:N:447:TYR:HB2	1.77	0.50
2:B:184:LEU:HD23	2:B:185:MET:N	2.27	0.50
4:D:35:ALA:HB3	27:D:4135:HOH:O	2.12	0.50
6:F:48:LEU:O	6:F:50:PRO:HD3	2.11	0.50
1:N:302:ARG:NH1	2:O:84:LEU:HD11	2.26	0.50
25:C:264:PEK:H71	25:C:264:PEK:H32	1.94	0.50
2:O:164:ALA:O	2:O:194:GLY:HA3	2.12	0.50
9:V:67:GLY:HA2	27:V:3310:HOH:O	2.12	0.50
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.10	0.50
2:B:146:MET:SD	2:B:189:PRO:HB3	2.52	0.50
2:B:79:PRO:O	2:B:83:ILE:HG13	2.10	0.50
3:C:47:LEU:O	3:C:51:MET:HG2	2.12	0.50
8:H:46:LYS:HZ3	8:U:55:TRP:HB2	1.75	0.50
1:N:472:ILE:HG21	18:Y:1522:TGL:HA91	1.91	0.50
2:O:22:HIS:CD2	2:O:26:HIS:CE1	2.99	0.50
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.93	0.50
2:O:65:TRP:HZ3	22:O:1230:PSC:H331	1.72	0.50
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.50
1:A:472:ILE:HG21	18:L:522:TGL:CA9	2.41	0.50
4:Q:78:TRP:O	4:Q:82:VAL:HG23	2.12	0.50
6:S:81:ARG:HG2	6:S:88:HIS:CD2	2.47	0.50
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.47	0.49
2:B:207:MET:O	2:B:207:MET:HG3	2.12	0.49
4:D:51:LEU:HB3	4:D:56:LYS:HG3	1.93	0.49
8:H:54:GLU:OE1	8:H:54:GLU:HA	2.11	0.49
27:E:2292:HOH:O	9:I:4:LEU:HD13	2.11	0.49
13:Z:23:PHE:O	13:Z:27:LEU:HG	2.12	0.49
23:B:1086:CHD:H20	7:T:18:PHE:CD2	2.47	0.49
23:B:1086:CHD:H212	23:B:1086:CHD:H12	1.94	0.49
22:B:230:PSC:H12	22:B:230:PSC:H322	1.94	0.49
5:E:6:GLU:HB2	5:E:10:GLU:OE1	2.12	0.49
5:E:52:LEU:O	5:E:55:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:GLU:O	6:F:65:ASP:HB2	2.12	0.49
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.94	0.49
1:N:309:THR:HG22	17:N:516:HEA:HMB2	1.92	0.49
1:N:35:LEU:CD1	1:N:462:LEU:HD13	2.42	0.49
7:T:38:HIS:CE1	26:T:1269:CDL:H111	2.47	0.49
1:A:15:ILE:HG21	1:A:98:ASN:ND2	2.27	0.49
8:H:36:PHE:HB2	8:H:56:TYR:HB2	1.94	0.49
3:P:157:LYS:HZ2	25:P:1265:PEK:H052	1.77	0.49
1:A:337:ALA:HB2	1:A:394:VAL:CG2	2.42	0.49
2:B:33:LEU:O	2:B:37:LEU:HB2	2.13	0.49
7:G:8:HIS:HD2	25:G:1263:PEK:H232	1.78	0.49
19:N:1524:PGV:H152	19:N:1524:PGV:H301	1.94	0.49
1:N:293:PHE:CE1	1:N:361:SER:HB3	2.48	0.49
1:N:5:ARG:O	1:N:9:SER:HB2	2.12	0.49
2:O:134:ARG:HG2	2:O:135:LEU:HG	1.94	0.49
3:P:57:TRP:O	3:P:57:TRP:HD1	1.96	0.49
1:N:507:GLU:HG3	3:P:5:THR:OG1	2.12	0.49
1:A:17:THR:OG1	18:L:522:TGL:H281	2.11	0.49
1:N:115:SER:HB3	1:N:145:LEU:HB2	1.94	0.49
3:P:134:THR:HA	3:P:249:TRP:HE1	1.77	0.49
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.13	0.49
6:S:33:ILE:HG22	6:S:34:LEU:HD23	1.95	0.49
10:W:8:LYS:O	10:W:12:PHE:HD1	1.96	0.49
18:Y:1522:TGL:OA1	18:Y:1522:TGL:HC21	2.12	0.49
22:O:1230:PSC:H12	22:O:1230:PSC:H322	1.95	0.49
3:P:158:HIS:NE2	25:P:1265:PEK:H051	2.28	0.49
1:N:514:LYS:NZ	27:N:3395:HOH:O	2.43	0.49
1:A:68:PHE:CE2	1:A:109:PHE:HA	2.47	0.49
2:B:125:THR:HG23	2:B:134:ARG:HG3	1.93	0.49
12:L:20:ARG:HH22	18:L:522:TGL:HC61	1.78	0.49
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.93	0.49
2:O:95:LEU:HG	2:O:96:THR:N	2.28	0.49
3:P:219:PHE:O	3:P:222:GLN:HB3	2.13	0.49
10:W:56:PRO:HD3	12:Y:46:LYS:HE3	1.93	0.49
1:N:339:MET:HE1	18:N:1523:TGL:HB62	1.95	0.48
17:N:516:HEA:H241	2:O:72:ILE:HG22	1.94	0.48
3:P:225:PHE:N	3:P:225:PHE:CD1	2.81	0.48
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.47	0.48
12:L:24:MET:SD	18:L:522:TGL:H162	2.53	0.48
4:Q:129:ALA:HB1	4:Q:133:GLY:HA3	1.96	0.48
3:P:128:GLU:OE1	7:T:38:HIS:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.95	0.48
2:B:56:MET:HA	22:B:230:PSC:H202	1.94	0.48
4:D:121:LYS:HG2	11:K:53:TRP:CD1	2.48	0.48
1:N:443:TYR:CD1	1:N:447:TYR:HB2	2.49	0.48
1:A:248:LEU:HB2	1:A:249:PRO:HD3	1.94	0.48
3:C:225:PHE:HA	27:C:2236:HOH:O	2.13	0.48
1:N:65:MET:HB3	17:N:515:HEA:CAC	2.42	0.48
9:I:37:PHE:CD1	9:I:38:ALA:N	2.82	0.48
7:T:31:CYS:SG	26:T:1269:CDL:H552	2.53	0.48
1:N:5:ARG:HB2	12:Y:3:TYR:CE1	2.49	0.48
1:A:476:PHE:CD2	12:L:15:VAL:HG11	2.49	0.48
22:B:230:PSC:H142	22:B:230:PSC:C34	2.31	0.48
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	1.95	0.48
2:O:57:ASP:H	22:O:1230:PSC:C20	2.19	0.48
2:O:69:PRO:HA	2:O:72:ILE:HD12	1.95	0.48
1:N:510:TYR:CG	6:S:49:VAL:HG13	2.48	0.48
7:T:84:LYS:CD	7:T:84:LYS:H	2.19	0.48
22:O:1230:PSC:H072	9:V:10:ARG:HE	1.77	0.48
2:B:143:VAL:HB	2:B:222:TRP:CZ3	2.49	0.48
2:B:155:SER:OG	2:B:156:SER:N	2.46	0.48
2:B:100:MET:CE	2:B:157:GLU:HG3	2.44	0.48
2:B:95:LEU:HD12	2:B:96:THR:H	1.79	0.48
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.67	0.48
5:R:14:ARG:HB3	5:R:14:ARG:HH11	1.79	0.48
1:A:361:SER:O	1:A:365:ILE:HG12	2.13	0.48
1:A:383:MET:HE2	1:A:421:VAL:HB	1.96	0.48
2:B:188:ARG:HB3	2:B:189:PRO:HD2	1.96	0.48
3:C:144:ILE:HG13	3:C:166:THR:HG21	1.96	0.48
3:C:187:THR:HG22	25:C:264:PEK:H052	1.96	0.48
23:C:271:CHD:H222	23:C:271:CHD:H162	1.53	0.48
1:N:94:PHE:HB3	19:N:1266:PGV:O11	2.14	0.48
1:N:66:ILE:HG23	1:N:246:LEU:HD21	1.96	0.48
2:O:66:THR:HG22	2:O:67:ILE:N	2.28	0.48
3:P:149:HIS:HA	3:P:152:MET:HE2	1.96	0.48
1:A:161:ALA:HB1	1:A:192:ALA:O	2.14	0.48
18:N:1523:TGL:HG32	27:Q:4216:HOH:O	2.12	0.48
2:O:52:HIS:ND1	5:R:40:ASP:HB2	2.28	0.48
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.13	0.48
1:A:397:PHE:HB3	1:A:398:PRO:HD3	1.96	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
2:B:121:TYR:O	2:B:138:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:PRO:O	7:G:29:ALA:HB3	2.14	0.47
1:N:513:LEU:O	1:N:514:LYS:HB2	2.13	0.47
3:P:4:GLN:NE2	3:P:6:HIS:O	2.43	0.47
7:T:8:HIS:HD2	25:T:263:PEK:H232	1.79	0.47
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.14	0.47
3:P:88:ILE:O	3:P:91:VAL:HB	2.14	0.47
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.97	0.47
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.95	0.47
19:A:524:PGV:H321	19:A:524:PGV:H152	1.96	0.47
3:C:198:PHE:O	25:C:264:PEK:H22	2.15	0.47
3:C:131:LEU:HD13	3:C:253:TYR:OH	2.14	0.47
8:H:49:ASP:O	8:H:52:VAL:HG22	2.14	0.47
1:N:468:MET:O	1:N:472:ILE:HG13	2.14	0.47
1:N:44:PRO:HB3	2:O:134:ARG:NH2	2.29	0.47
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.25	0.47
19:A:524:PGV:C15	19:A:524:PGV:H321	2.45	0.47
1:A:310:MET:O	2:B:73:LEU:HD13	2.14	0.47
3:C:149:HIS:HA	3:C:152:MET:HE2	1.95	0.47
6:F:96:LEU:HD23	6:F:97:ALA:N	2.29	0.47
18:L:522:TGL:H272	18:L:522:TGL:H231	1.96	0.47
17:A:515:HEA:H11	17:A:515:HEA:HMB1	1.70	0.47
1:A:357:VAL:HG22	2:B:27:THR:CG2	2.44	0.47
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.49	0.47
18:L:522:TGL:OA1	18:L:522:TGL:HC21	2.15	0.47
13:M:35:TYR:HD2	13:M:36:HIS:ND1	2.12	0.47
5:R:21:LYS:HE3	27:R:3128:HOH:O	2.13	0.47
8:U:49:ASP:O	8:U:52:VAL:HG22	2.14	0.47
11:X:47:ARG:HG3	11:X:48:VAL:N	2.29	0.47
1:A:104:LEU:HB2	1:A:156:SER:HB2	1.97	0.47
6:F:74:LEU:HD12	6:F:80:GLN:OE1	2.14	0.47
7:G:84:LYS:HD2	7:G:84:LYS:N	2.16	0.47
18:L:522:TGL:HA72	18:L:522:TGL:H211	1.97	0.47
2:O:65:TRP:CE3	22:O:1230:PSC:H331	2.50	0.47
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.50	0.47
19:N:1524:PGV:C15	19:N:1524:PGV:H321	2.44	0.47
5:R:43:PRO:HB2	5:R:48:ILE:CD1	2.42	0.47
26:C:270:CDL:C19	26:C:270:CDL:H642	2.35	0.47
8:H:55:TRP:O	8:H:59:VAL:HG23	2.14	0.47
1:A:132:LEU:HD12	1:A:132:LEU:O	2.15	0.47
7:G:3:ALA:O	7:G:4:ALA:HB2	2.15	0.47
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:157:LYS:HZ1	25:P:1265:PEK:H052	1.78	0.47
3:P:50:ASN:O	3:P:54:MET:HG3	2.14	0.47
3:C:67:PHE:N	3:C:67:PHE:CD2	2.82	0.47
1:N:164:PHE:O	1:N:168:ILE:HG13	2.15	0.47
1:N:376:HIS:HA	27:N:3228:HOH:O	2.14	0.47
4:Q:131:ILE:HG23	9:V:50:PHE:HB2	1.97	0.47
25:T:1264:PEK:H71	25:T:1264:PEK:C3	2.45	0.47
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.50	0.47
7:G:3:ALA:HB3	25:G:1263:PEK:H361	1.97	0.47
1:N:3:ILE:HG23	1:N:7:LEU:HD22	1.97	0.47
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.45	0.47
13:M:42:LYS:CE	13:M:42:LYS:HA	2.41	0.46
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.50	0.46
3:C:173:PHE:C	3:C:173:PHE:CD2	2.89	0.46
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.71	0.46
1:A:382:SER:CA	17:A:515:HEA:HMC2	2.43	0.46
2:B:185:MET:SD	2:B:185:MET:C	2.93	0.46
1:N:12:HIS:CE1	1:N:13:LYS:HG2	2.51	0.46
1:N:429:HIS:HB3	18:O:1521:TGL:HB41	1.96	0.46
8:U:28:ASN:ND2	27:U:3134:HOH:O	2.40	0.46
1:A:378:HIS:CG	1:A:425:PHE:CE2	3.03	0.46
1:N:211:THR:HG22	1:N:215:LEU:HD12	1.97	0.46
6:S:13:ALA:O	6:S:18:ARG:HD2	2.15	0.46
8:U:36:PHE:HB2	8:U:56:TYR:HB2	1.98	0.46
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.67	0.46
13:M:26:PHE:O	13:M:29:PRO:HD2	2.15	0.46
6:S:72:PHE:CE2	6:S:83:PRO:HD3	2.49	0.46
1:A:235:PHE:C	1:A:235:PHE:CD2	2.88	0.46
1:A:413:HIS:HE2	1:A:468:MET:HB2	1.79	0.46
3:C:51:MET:SD	26:C:270:CDL:C62	3.04	0.46
24:P:1272:DMU:H30	24:P:1272:DMU:O1	2.16	0.46
3:P:147:ALA:HB2	3:P:162:ALA:CB	2.46	0.46
3:P:59:ARG:HG3	26:P:1270:CDL:H512	1.96	0.46
1:A:140:GLY:O	1:A:213:ARG:NH2	2.49	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.51	0.46
7:G:2:SER:OG	25:G:1263:PEK:H301	2.16	0.46
19:P:1267:PGV:H181	26:P:1270:CDL:H812	1.96	0.46
1:A:346:PHE:CD2	1:A:347:LEU:HD23	2.50	0.46
12:L:11:ILE:HG13	12:L:13:PHE:O	2.16	0.46
7:T:70:PHE:O	25:T:1264:PEK:N	2.48	0.46
8:H:46:LYS:HE2	27:H:4276:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:417:MET:O	1:N:421:VAL:HG22	2.16	0.46
19:P:1267:PGV:H182	26:P:1270:CDL:C67	2.45	0.46
17:A:515:HEA:H261	17:A:515:HEA:H171	1.72	0.46
19:A:525:PGV:H21	3:C:57:TRP:CZ2	2.51	0.46
3:C:112:LEU:HA	7:G:52:HIS:CD2	2.50	0.46
7:T:11:TPO:O	7:T:11:TPO:CG2	2.64	0.46
27:C:4266:HOH:O	25:T:263:PEK:H042	2.15	0.46
1:A:395:HIS:HD2	1:A:396:TRP:CD2	2.34	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
2:B:217:LYS:HD3	2:B:217:LYS:HA	1.79	0.45
3:C:156:ARG:HE	23:C:271:CHD:H232	1.80	0.45
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.98	0.45
18:N:1523:TGL:H271	2:O:46:LEU:HD12	1.97	0.45
12:Y:24:MET:HE1	18:Y:1522:TGL:HC82	1.99	0.45
1:A:377:PHE:HE2	1:A:378:HIS:CE1	2.34	0.45
25:C:265:PEK:H041	6:F:1:ALA:N	2.32	0.45
12:L:20:ARG:HH12	18:L:522:TGL:CC6	2.16	0.45
2:O:72:ILE:HG13	27:O:4128:HOH:O	2.15	0.45
3:P:173:PHE:CD2	3:P:173:PHE:C	2.88	0.45
23:W:1060:CHD:H161	23:W:1060:CHD:H212	1.84	0.45
19:A:525:PGV:H251	19:A:525:PGV:H42	1.98	0.45
2:B:22:HIS:NE2	2:B:26:HIS:NE2	2.64	0.45
1:A:21:LEU:HD23	18:L:522:TGL:H221	1.98	0.45
1:N:230:LEU:HD21	3:P:100:ALA:HA	1.97	0.45
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.97	0.45
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.97	0.45
2:B:22:HIS:CD2	2:B:26:HIS:CE1	3.04	0.45
23:G:86:CHD:H212	23:G:86:CHD:H12	1.97	0.45
13:M:34:LEU:HA	13:M:34:LEU:HD12	1.68	0.45
1:N:367:LEU:CD2	1:N:433:LEU:HD23	2.46	0.45
26:T:1269:CDL:C52	26:T:1269:CDL:H202	2.40	0.45
1:A:115:SER:HA	1:A:145:LEU:HD12	1.99	0.45
1:A:248:LEU:O	1:A:251:PHE:HB2	2.15	0.45
25:C:265:PEK:H371	26:G:269:CDL:H273	1.99	0.45
1:N:450:TRP:CE3	1:N:453:ILE:HD12	2.52	0.45
1:N:309:THR:CG2	17:N:516:HEA:HMB2	2.47	0.45
2:O:62:GLU:O	2:O:66:THR:HB	2.16	0.45
2:O:69:PRO:HG3	22:O:1230:PSC:H183	1.98	0.45
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.32	0.45
1:A:443:TYR:CD1	1:A:447:TYR:HB2	2.50	0.45
1:A:513:LEU:O	1:A:514:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:HIS:CE1	2:B:200:CYS:HB2	2.52	0.45
2:B:215:PRO:HD3	9:I:60:PHE:CD2	2.52	0.45
2:B:131:GLY:O	4:D:122:ARG:HD3	2.16	0.45
7:G:44:ARG:HA	7:G:45:PRO:HD2	1.83	0.45
1:N:195:LEU:HG	1:N:245:ILE:CD1	2.42	0.45
1:N:397:PHE:N	1:N:398:PRO:CD	2.78	0.45
1:N:313:ALA:CB	17:N:516:HEA:H262	2.46	0.45
7:T:70:PHE:HD1	25:T:1264:PEK:O11	2.00	0.45
1:A:443:TYR:N	1:A:443:TYR:CD2	2.85	0.45
2:B:14:SER:O	2:B:18:GLU:HG3	2.16	0.45
2:B:97:VAL:O	2:B:152:MET:HE3	2.17	0.45
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.74	0.45
2:B:41:ILE:CD1	22:B:230:PSC:H342	2.47	0.45
2:B:78:LEU:HD12	26:T:1269:CDL:C35	2.47	0.45
3:C:112:LEU:HB3	3:C:118:PRO:HB3	1.98	0.45
23:J:60:CHD:H161	23:J:60:CHD:H212	1.79	0.45
4:D:145:TRP:CZ3	11:K:45:VAL:HG22	2.52	0.45
3:P:160:LEU:HD21	3:P:222:GLN:HG3	1.99	0.45
26:T:1269:CDL:H222	26:T:1269:CDL:H251	1.84	0.45
3:C:163:LEU:HD23	3:C:219:PHE:HA	1.99	0.45
3:C:16:TRP:HB2	3:C:17:PRO:HD3	1.98	0.45
4:D:95:LEU:HD21	13:M:27:LEU:CD1	2.47	0.45
26:G:269:CDL:H222	26:G:269:CDL:H251	1.86	0.45
1:N:460:ILE:HA	4:Q:92:THR:HG21	1.98	0.45
1:N:8:PHE:N	1:N:8:PHE:CD1	2.85	0.45
2:O:32:PHE:HE2	18:O:1521:TGL:HB91	1.80	0.45
6:S:92:VAL:HG23	6:S:92:VAL:O	2.16	0.45
8:U:37:HIS:CD2	8:U:76:ARG:CZ	2.99	0.45
2:B:68:LEU:HB3	22:B:230:PSC:H182	1.99	0.45
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.69	0.45
26:G:269:CDL:H271	1:N:282:PHE:HE2	1.81	0.45
12:L:33:PHE:O	12:L:36:PRO:HD2	2.16	0.45
18:N:1523:TGL:CC2	18:N:1523:TGL:HG11	2.41	0.45
2:O:22:HIS:NE2	2:O:26:HIS:HE1	2.06	0.45
1:A:302:ARG:NH1	27:A:4150:HOH:O	2.49	0.45
1:N:467:LEU:O	1:N:470:PHE:HB3	2.17	0.45
1:N:91:ASP:OD1	1:N:95:PRO:HB3	2.15	0.45
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.99	0.45
12:Y:11:ILE:HD12	12:Y:13:PHE:CE1	2.51	0.45
26:C:270:CDL:H171	26:C:270:CDL:H202	1.77	0.44
1:N:151:HIS:CD2	25:T:1264:PEK:H382	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:6:VAL:HA	6:S:7:PRO:HD2	1.87	0.44
1:N:220:PHE:CE1	1:N:231:TYR:HB2	2.52	0.44
1:N:507:GLU:OE1	6:S:51:SER:HA	2.18	0.44
2:O:116:LEU:HD12	2:O:117:SER:N	2.33	0.44
2:O:161:HIS:CE1	2:O:200:CYS:CB	3.01	0.44
25:P:1265:PEK:H371	26:T:1269:CDL:H261	1.99	0.44
12:Y:36:PRO:O	12:Y:40:VAL:HG23	2.17	0.44
1:A:449:MET:SD	2:B:5:MET:CG	3.05	0.44
2:B:12:ALA:HB3	9:I:47:TYR:CE2	2.53	0.44
3:C:81:TYR:O	3:C:85:LEU:HG	2.18	0.44
1:N:381:LEU:HB3	17:N:515:HEA:CB	2.46	0.44
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.72	0.44
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.83	0.44
7:T:3:ALA:O	7:T:4:ALA:HB2	2.16	0.44
7:T:8:HIS:CD2	25:T:263:PEK:H232	2.53	0.44
18:Y:1522:TGL:C23	18:Y:1522:TGL:H272	2.47	0.44
1:A:424:THR:OG1	1:A:458:SER:N	2.51	0.44
1:A:439:ARG:HH21	17:A:515:HEA:CGD	2.30	0.44
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.53	0.44
1:N:12:HIS:CD2	1:N:91:ASP:HA	2.53	0.44
22:O:1230:PSC:C34	22:O:1230:PSC:H142	2.32	0.44
3:P:156:ARG:HE	23:P:1271:CHD:C23	2.30	0.44
2:O:12:ALA:HB3	9:V:47:TYR:CE2	2.53	0.44
1:A:397:PHE:N	1:A:398:PRO:CD	2.80	0.44
1:A:35:LEU:CD1	1:A:462:LEU:HD13	2.48	0.44
1:A:96:ARG:NH2	3:C:61:VAL:HG22	2.32	0.44
4:D:32:ASN:HA	4:D:32:ASN:HD22	1.64	0.44
6:F:92:VAL:O	6:F:92:VAL:CG2	2.62	0.44
1:A:6:TRP:HH2	12:L:10:ASN:O	2.01	0.44
1:N:314:ILE:O	1:N:318:VAL:HG23	2.18	0.44
7:T:17:ARG:HD2	27:T:3309:HOH:O	2.17	0.44
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.86	0.44
1:N:473:TRP:NE1	12:Y:22:LEU:HB2	2.32	0.44
1:A:397:PHE:HD1	1:A:405:LEU:HG	1.83	0.44
7:G:79:PRO:HD2	27:G:2136:HOH:O	2.17	0.44
18:N:1523:TGL:HC22	18:N:1523:TGL:HC51	1.78	0.44
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.99	0.44
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.74	0.44
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.99	0.44
4:Q:11:TYR:CD1	4:Q:12:ALA:N	2.86	0.44
2:O:131:GLY:O	4:Q:122:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.98	0.44
1:A:98:ASN:HA	27:A:2052:HOH:O	2.17	0.44
2:B:159:VAL:HG23	2:B:160:LEU:N	2.32	0.44
22:B:230:PSC:H032	27:E:2129:HOH:O	2.17	0.44
22:B:230:PSC:H241	22:B:230:PSC:H62	2.00	0.44
5:E:71:VAL:HG11	5:E:85:VAL:HG11	1.98	0.44
7:G:11:TPO:CG2	7:G:11:TPO:O	2.66	0.44
26:G:269:CDL:H601	26:G:269:CDL:H571	1.48	0.44
1:N:361:SER:O	1:N:365:ILE:HG12	2.17	0.44
4:Q:131:ILE:HG23	9:V:50:PHE:CB	2.48	0.44
8:U:39:CYS:O	8:U:43:MET:HG2	2.17	0.44
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.53	0.44
1:A:397:PHE:CD1	1:A:405:LEU:HG	2.53	0.44
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.83	0.44
5:E:19:PHE:O	5:E:57:ARG:NH2	2.51	0.44
8:H:37:HIS:CD2	8:H:76:ARG:CZ	3.01	0.44
1:N:395:HIS:O	1:N:398:PRO:HD2	2.18	0.44
4:D:23:PRO:O	4:D:25:PRO:HD3	2.18	0.43
4:D:48:TRP:O	4:D:51:LEU:HB2	2.18	0.43
8:H:9:LYS:O	8:H:10:ASN:CB	2.66	0.43
26:P:1270:CDL:H632	26:P:1270:CDL:H602	1.76	0.43
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.18	0.43
4:D:20:ARG:HG3	4:D:20:ARG:H	1.66	0.43
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.99	0.43
8:H:28:ASN:ND2	27:H:2134:HOH:O	2.50	0.43
1:N:499:PRO:HD2	12:Y:7:PRO:HD3	1.99	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.87	0.43
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.18	0.43
5:R:100:THR:OG1	5:R:103:GLU:HG3	2.17	0.43
8:U:49:ASP:OD1	8:U:51:SER:HB3	2.18	0.43
1:A:368:HIS:O	1:A:370:THR:HG23	2.18	0.43
18:A:523:TGL:H242	18:A:523:TGL:H212	1.78	0.43
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.74	0.43
4:D:42:GLU:OE2	4:D:45:LYS:HE2	2.18	0.43
1:N:9:SER:HB3	27:N:4019:HOH:O	2.18	0.43
2:O:161:HIS:CE1	2:O:200:CYS:HB2	2.53	0.43
2:O:23:PHE:HE2	2:O:79:PRO:HG2	1.82	0.43
8:U:57:ARG:O	8:U:61:LYS:HB2	2.18	0.43
1:A:377:PHE:HB2	17:A:516:HEA:HMD3	2.01	0.43
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.18	0.43
1:A:440:TYR:HE2	2:B:204:HIS:CE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:OD2	4:D:19:ARG:HD3	2.19	0.43
22:O:1230:PSC:H221	22:O:1230:PSC:H251	1.77	0.43
2:O:184:LEU:HD23	2:O:185:MET:N	2.33	0.43
2:O:29:MET:HB2	9:V:35:TYR:CE2	2.53	0.43
3:P:198:PHE:O	25:T:1264:PEK:H22	2.19	0.43
1:A:186:TRP:O	1:A:189:MET:N	2.52	0.43
1:A:325:ALA:HA	22:B:230:PSC:H291	1.99	0.43
26:C:270:CDL:H602	26:C:270:CDL:H632	1.81	0.43
5:E:105:GLY:O	5:E:108:LYS:HE2	2.17	0.43
1:N:109:PHE:CE2	1:N:112:LEU:HD22	2.53	0.43
17:N:515:HEA:H122	17:N:515:HEA:HHC	2.00	0.43
25:G:1263:PEK:C9	3:P:244:PHE:HA	2.47	0.43
9:V:47:TYR:HB2	27:V:4249:HOH:O	2.19	0.43
1:A:440:TYR:CE2	2:B:205:SER:HA	2.53	0.43
1:A:302:ARG:NH1	2:B:84:LEU:HD11	2.34	0.43
1:N:131:PRO:HG2	2:O:159:VAL:HA	2.00	0.43
7:T:31:CYS:SG	26:T:1269:CDL:C55	3.07	0.43
10:W:50:LEU:HD22	10:W:50:LEU:O	2.18	0.43
1:A:104:LEU:C	1:A:107:PRO:HD2	2.39	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.01	0.43
1:N:450:TRP:HE3	1:N:453:ILE:HD12	1.83	0.43
1:N:498:CYS:HA	1:N:499:PRO:HA	1.74	0.43
5:R:14:ARG:NH1	5:R:14:ARG:HB3	2.33	0.43
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.78	0.43
1:N:51:ASP:HB2	2:O:202:SER:O	2.19	0.43
4:Q:60:TYR:OH	4:Q:67:SER:HA	2.19	0.43
5:R:40:ASP:CG	9:V:11:GLY:HA2	2.39	0.43
1:A:35:LEU:HD11	1:A:462:LEU:HD13	2.01	0.43
6:F:14:THR:OG1	6:F:15:GLY:N	2.51	0.43
2:O:190:GLY:HA3	27:O:4222:HOH:O	2.18	0.43
2:O:3:TYR:CE1	2:O:6:GLN:HG3	2.54	0.43
26:T:1269:CDL:H141	27:T:4142:HOH:O	2.17	0.43
1:A:293:PHE:HB2	1:A:364:ASP:OD1	2.19	0.43
1:A:65:MET:HB3	17:A:515:HEA:HAC	2.00	0.43
25:C:265:PEK:H382	1:N:279:SER:OG	2.19	0.43
1:A:344:PHE:CD1	1:A:344:PHE:C	2.92	0.42
2:B:12:ALA:HB3	9:I:47:TYR:HE2	1.84	0.42
7:G:23:LEU:C	7:G:26:PRO:HD2	2.39	0.42
1:N:243:VAL:HA	1:N:246:LEU:HD12	1.99	0.42
1:N:75:ILE:O	1:N:79:GLY:HA3	2.18	0.42
2:O:188:ARG:HB3	2:O:189:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1265:PEK:H21	27:P:4191:HOH:O	2.19	0.42
4:Q:102:TYR:HD1	13:Z:35:TYR:HE1	1.67	0.42
6:S:87:THR:HG22	27:S:3350:HOH:O	2.18	0.42
1:A:176:MET:HG3	1:A:180:GLN:HB3	2.00	0.42
1:A:324:LEU:HD13	2:B:41:ILE:CG2	2.48	0.42
2:B:13:THR:O	2:B:187:SER:HB2	2.19	0.42
17:N:516:HEA:H241	2:O:72:ILE:HG21	1.98	0.42
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.49	0.42
2:B:59:GLN:NE2	25:P:1265:PEK:O04	2.52	0.42
4:Q:109:HIS:C	4:Q:111:PHE:H	2.22	0.42
1:A:278:MET:HB3	7:T:5:LYS:HD3	2.02	0.42
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.83	0.42
8:H:9:LYS:HB3	8:H:10:ASN:H	1.52	0.42
8:H:65:PRO:O	8:H:69:VAL:HG23	2.19	0.42
2:O:108:TYR:CE1	2:O:142:VAL:CG2	3.02	0.42
2:O:216:LEU:HB3	27:O:4168:HOH:O	2.18	0.42
2:O:22:HIS:CD2	2:O:26:HIS:HE1	2.38	0.42
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.76	0.42
26:P:1270:CDL:HB22	26:P:1270:CDL:PA1	2.59	0.42
3:P:241:TYR:O	3:P:244:PHE:HB3	2.19	0.42
1:A:35:LEU:HD11	1:A:462:LEU:HB2	2.01	0.42
4:D:102:TYR:CD1	13:M:35:TYR:CE1	3.04	0.42
4:D:124:LEU:O	4:D:140:TYR:OH	2.30	0.42
23:P:1271:CHD:H222	23:P:1271:CHD:H162	1.54	0.42
3:P:198:PHE:CD2	25:T:1264:PEK:C03	3.02	0.42
3:P:57:TRP:O	3:P:61:VAL:HG23	2.19	0.42
1:A:484:THR:HG22	27:A:4238:HOH:O	2.18	0.42
2:B:41:ILE:HD13	22:B:230:PSC:H342	2.01	0.42
7:G:30:LEU:CD1	26:G:269:CDL:H252	2.49	0.42
1:N:325:ALA:O	1:N:328:HIS:HB3	2.20	0.42
1:N:416:ILE:CG2	1:N:464:ALA:HB2	2.49	0.42
2:O:99:THR:HG22	2:O:152:MET:CE	2.49	0.42
27:N:4241:HOH:O	2:O:58:ALA:HB3	2.20	0.42
5:R:5:HIS:HB3	5:R:6:GLU:H	1.67	0.42
5:R:61:PHE:HE1	5:R:98:ILE:HA	1.83	0.42
6:S:74:LEU:HD11	6:S:89:TYR:O	2.19	0.42
7:T:38:HIS:NE2	26:T:1269:CDL:HA21	2.34	0.42
2:O:146:MET:CE	9:V:56:SER:HB2	2.49	0.42
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.94	0.42
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.00	0.42
2:B:138:VAL:HG22	2:B:210:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:THR:CG2	2:B:67:ILE:N	2.80	0.42
3:C:244:PHE:HA	25:T:263:PEK:H9	2.01	0.42
26:C:270:CDL:HB22	26:C:270:CDL:PA1	2.59	0.42
4:D:109:HIS:C	4:D:111:PHE:H	2.22	0.42
12:L:25:MET:HG2	18:L:522:TGL:HA62	2.02	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.54	0.42
2:O:37:LEU:HD12	2:O:37:LEU:HA	1.89	0.42
6:S:76:LYS:HE2	6:S:93:PRO:HG3	1.99	0.42
1:A:231:TYR:C	1:A:231:TYR:CD1	2.92	0.42
1:A:258:VAL:HG13	1:A:327:LEU:CD2	2.50	0.42
2:B:3:TYR:CE1	2:B:6:GLN:HG3	2.54	0.42
4:D:94:LEU:HD23	11:K:28:VAL:CG2	2.50	0.42
5:E:52:LEU:HA	5:E:52:LEU:HD23	1.87	0.42
1:N:62:ALA:HB3	1:N:126:TRP:HB3	2.01	0.42
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.54	0.42
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.88	0.42
4:Q:130:PRO:HG2	4:Q:131:ILE:CD1	2.49	0.42
6:S:57:ILE:HG13	6:S:73:TRP:CZ3	2.55	0.42
7:T:2:SER:O	7:T:3:ALA:HB3	2.20	0.42
2:B:155:SER:O	2:B:174:ALA:HB1	2.19	0.42
3:C:187:THR:HA	25:C:264:PEK:O12	2.20	0.42
1:A:104:LEU:HD23	3:C:21:ALA:HA	2.02	0.42
3:C:30:GLY:HA2	3:C:42:LEU:HB3	2.02	0.42
26:G:269:CDL:OA7	26:G:269:CDL:H342	2.19	0.42
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.67	0.42
10:J:36:MET:O	10:J:40:LEU:HG	2.20	0.42
17:N:516:HEA:HMB1	17:N:516:HEA:H11	1.86	0.42
2:O:143:VAL:HG12	2:O:219:PHE:HD1	1.84	0.42
2:O:84:LEU:HD12	2:O:87:MET:HE2	2.00	0.42
1:A:446:ALA:HB1	2:B:3:TYR:C	2.41	0.42
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.85	0.42
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.51	0.42
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.54	0.42
13:Z:6:ALA:O	13:Z:9:PRO:HD3	2.20	0.42
1:A:325:ALA:O	1:A:328:HIS:HB3	2.20	0.42
25:C:265:PEK:H371	26:G:269:CDL:C27	2.50	0.42
1:N:242:GLU:O	1:N:246:LEU:HG	2.20	0.42
1:N:378:HIS:CG	1:N:425:PHE:CE2	3.08	0.42
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.55	0.42
3:P:132:LEU:O	3:P:136:VAL:HG23	2.20	0.42
5:R:84:TYR:CZ	5:R:88:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:24:ALA:O	7:T:27:SER:HB2	2.19	0.42
3:C:68:GLN:HB2	3:C:70:HIS:CD2	2.55	0.41
4:D:24:LEU:HD12	5:E:30:ARG:HA	2.02	0.41
5:E:89:LEU:O	5:E:93:LEU:HG	2.20	0.41
5:E:49:ASP:OD2	5:E:92:THR:HG21	2.20	0.41
7:G:25:LEU:HA	7:G:25:LEU:HD23	1.76	0.41
3:C:128:GLU:OE1	7:G:38:HIS:HB3	2.20	0.41
11:K:32:MET:HE2	11:K:32:MET:HB3	2.01	0.41
2:O:135:LEU:O	2:O:208:PRO:HG3	2.19	0.41
2:O:224:ALA:O	2:O:227:LEU:CG	2.65	0.41
3:P:60:ASP:HA	3:P:63:ARG:HD2	2.02	0.41
4:Q:130:PRO:O	4:Q:136:ALA:HB2	2.20	0.41
4:Q:84:ALA:O	4:Q:88:PHE:HD1	2.03	0.41
8:U:43:MET:HE3	8:U:43:MET:HB3	1.88	0.41
3:C:67:PHE:HA	10:J:9:GLN:HG2	2.03	0.41
12:L:46:LYS:O	12:L:47:LYS:HB2	2.20	0.41
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.20	0.41
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.91	0.41
3:P:41:THR:O	3:P:44:MET:HB2	2.20	0.41
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.41
4:D:77:GLU:HA	11:K:10:HIS:CD2	2.55	0.41
1:N:258:VAL:HG13	1:N:327:LEU:CD2	2.51	0.41
4:Q:34:SER:OG	4:Q:37:GLN:HG3	2.20	0.41
1:A:243:VAL:HB	17:A:516:HEA:CAC	2.50	0.41
3:C:231:HIS:CG	19:C:267:PGV:H061	2.55	0.41
8:H:27:ARG:O	8:H:31:GLN:N	2.44	0.41
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.81	0.41
10:J:45:TYR:O	10:J:48:TYR:HB3	2.20	0.41
18:N:1523:TGL:H212	18:N:1523:TGL:H242	1.79	0.41
1:A:197:LEU:HB2	1:A:285:PHE:CZ	2.56	0.41
1:A:307:SER:HB3	26:T:1269:CDL:H182	2.02	0.41
1:A:425:PHE:HZ	17:A:515:HEA:C2B	2.34	0.41
1:A:512:ASN:HB3	6:F:38:ALA:HB2	2.01	0.41
3:C:146:TRP:CE3	3:C:162:ALA:HB2	2.56	0.41
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.95	0.41
2:O:175:ILE:HA	2:O:176:PRO:HD2	1.82	0.41
2:O:79:PRO:O	2:O:83:ILE:HG13	2.20	0.41
3:P:231:HIS:CG	19:P:1267:PGV:H061	2.56	0.41
3:P:30:GLY:CA	3:P:42:LEU:HB3	2.49	0.41
4:Q:87:PHE:C	4:Q:87:PHE:CD2	2.94	0.41
5:R:9:GLU:CD	5:R:9:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:50:VAL:HG12	8:U:50:VAL:O	2.20	0.41
2:O:207:MET:HG3	2:O:207:MET:O	2.21	0.41
3:P:108:PRO:HA	27:P:3207:HOH:O	2.20	0.41
3:P:42:LEU:HA	3:P:42:LEU:HD23	1.83	0.41
7:T:31:CYS:O	7:T:35:SER:HB2	2.21	0.41
12:Y:20:ARG:NH1	12:Y:20:ARG:HB3	2.36	0.41
1:A:184:PHE:O	1:A:188:VAL:HG23	2.21	0.41
19:A:525:PGV:H182	3:C:28:THR:HG22	2.02	0.41
2:B:146:MET:HG2	2:B:214:VAL:O	2.21	0.41
1:N:105:LEU:HA	1:N:108:SER:HB3	2.02	0.41
1:N:440:TYR:HE1	2:O:195:GLN:NE2	2.17	0.41
1:N:443:TYR:N	1:N:443:TYR:CD2	2.88	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.41
3:P:224:LYS:C	3:P:225:PHE:HD1	2.24	0.41
1:A:94:PHE:HB3	19:A:525:PGV:O11	2.21	0.41
3:C:138:LEU:HA	3:C:138:LEU:HD23	1.93	0.41
7:G:3:ALA:CB	25:G:1263:PEK:H382	2.40	0.41
7:G:33:LEU:HD22	7:G:33:LEU:HA	1.88	0.41
8:H:67:SER:HA	8:H:70:SER:HB3	2.03	0.41
1:N:161:ALA:HB1	1:N:192:ALA:O	2.20	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.56	0.41
3:P:205:GLY:O	3:P:208:VAL:HB	2.21	0.41
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.02	0.41
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.83	0.41
4:D:38:LYS:HE2	27:D:4155:HOH:O	2.21	0.41
6:F:72:PHE:CE2	6:F:83:PRO:HD3	2.56	0.41
2:O:12:ALA:HB3	9:V:47:TYR:HE2	1.84	0.41
3:P:103:HIS:HA	19:P:1268:PGV:O04	2.21	0.41
4:Q:31:LYS:HB3	27:Q:4171:HOH:O	2.20	0.41
1:N:262:SER:HA	1:N:332:ILE:HD13	2.03	0.41
1:N:381:LEU:HD23	1:N:381:LEU:HA	1.92	0.41
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.21	0.41
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.39	0.41
3:P:60:ASP:O	3:P:64:GLU:HG3	2.21	0.41
5:R:86:ILE:HD13	5:R:86:ILE:HA	1.96	0.41
6:S:82:CYS:HA	6:S:83:PRO:HD3	1.93	0.41
5:R:12:ASP:CG	9:V:10:ARG:HH22	2.24	0.41
12:Y:11:ILE:HG22	18:Y:1522:TGL:H271	2.02	0.41
12:Y:13:PHE:CA	18:Y:1522:TGL:HC31	2.38	0.41
1:A:403:TYR:CD1	1:A:479:LYS:HA	2.56	0.41
4:D:130:PRO:O	4:D:136:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:53:ARG:O	5:E:57:ARG:HG3	2.21	0.41
1:N:150:LEU:HD23	1:N:150:LEU:HA	1.81	0.41
4:Q:94:LEU:CD2	11:X:28:VAL:HG21	2.49	0.41
1:A:189:MET:HB3	1:A:189:MET:HE3	1.98	0.40
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.84	0.40
1:A:202:LEU:HB2	1:A:238:PHE:CG	2.56	0.40
1:A:313:ALA:HB3	2:B:73:LEU:HD11	2.02	0.40
1:A:378:HIS:CD2	1:A:425:PHE:CE2	3.08	0.40
1:A:402:GLY:O	1:A:482:VAL:HG23	2.21	0.40
22:B:230:PSC:H072	9:I:10:ARG:NH2	2.30	0.40
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.40
3:C:188:ILE:HG22	25:C:264:PEK:O13	2.21	0.40
23:J:60:CHD:H112	23:J:60:CHD:H12A	1.88	0.40
1:N:58:VAL:HG13	17:N:515:HEA:HBA1	2.02	0.40
4:Q:51:LEU:HB3	4:Q:56:LYS:HG3	2.03	0.40
3:C:248:VAL:HG22	25:T:263:PEK:H15	2.02	0.40
1:A:19:TYR:CG	1:A:76:GLY:HA3	2.55	0.40
1:A:132:LEU:HD23	2:B:199:ILE:HG23	2.03	0.40
3:C:250:LEU:HA	3:C:250:LEU:HD23	1.66	0.40
5:E:54:ALA:O	5:E:58:LEU:HD12	2.20	0.40
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.56	0.40
1:N:467:LEU:O	1:N:471:ILE:HG13	2.21	0.40
1:N:96:ARG:NH2	3:P:61:VAL:HG22	2.35	0.40
10:W:32:TYR:CD2	10:W:32:TYR:C	2.94	0.40
2:B:14:SER:HB3	2:B:168:LEU:HD22	2.04	0.40
3:C:157:LYS:HB3	3:C:157:LYS:HE2	1.93	0.40
3:C:59:ARG:O	3:C:63:ARG:HG3	2.21	0.40
5:E:37:VAL:HG11	5:E:70:VAL:HG21	2.03	0.40
7:G:8:HIS:HA	7:G:11:TPO:O1P	2.21	0.40
26:G:269:CDL:C27	1:N:282:PHE:HE2	2.35	0.40
13:M:37:LEU:O	13:M:40:TYR:HB2	2.21	0.40
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	2.03	0.40
2:O:191:LEU:HD23	2:O:191:LEU:HA	1.96	0.40
2:O:95:LEU:HD12	2:O:96:THR:H	1.86	0.40
11:X:43:SER:HA	11:X:44:PRO:HD3	1.91	0.40
2:B:175:ILE:HA	2:B:176:PRO:HD2	1.85	0.40
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.21	0.40
5:E:52:LEU:HD22	5:E:64:ALA:HB1	2.03	0.40
26:G:269:CDL:H421	1:N:311:ILE:HG13	2.04	0.40
1:N:243:VAL:HB	17:N:516:HEA:CAC	2.51	0.40
1:N:288:TRP:O	1:N:291:HIS:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:158:HIS:CE1	25:P:1265:PEK:H051	2.56	0.40
10:W:40:LEU:HD12	23:W:1060:CHD:H183	2.04	0.40
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.57	0.40
3:C:57:TRP:O	3:C:57:TRP:HD1	2.04	0.40
1:N:365:ILE:O	2:O:171:LYS:NZ	2.47	0.40
1:N:42:GLY:HA3	4:Q:104:TYR:HH	1.82	0.40
2:O:32:PHE:HD2	2:O:32:PHE:HA	1.79	0.40
3:P:109:THR:HA	27:P:4232:HOH:O	2.20	0.40
3:P:62:ILE:CD1	3:P:221:ARG:HD2	2.45	0.40
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.56	0.40
12:Y:9:LYS:HA	12:Y:9:LYS:HD3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	466 (91%)	42 (8%)	4 (1%)	19	43
1	N	512/514 (100%)	469 (92%)	40 (8%)	3 (1%)	25	50
2	B	225/227 (99%)	202 (90%)	20 (9%)	3 (1%)	12	30
2	O	225/227 (99%)	198 (88%)	21 (9%)	6 (3%)	5	12
3	C	257/261 (98%)	247 (96%)	9 (4%)	1 (0%)	34	60
3	P	257/261 (98%)	246 (96%)	10 (4%)	1 (0%)	34	60
4	D	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	80 (83%)	12 (12%)	4 (4%)	3	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	96/98 (98%)	83 (86%)	9 (9%)	4 (4%)	3	5
7	G	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	0	0
7	T	81/85 (95%)	61 (75%)	12 (15%)	8 (10%)	0	0
8	H	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	3	6
8	U	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	3	6
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	21
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	21
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	1 (2%)	1 (2%)	6	16
13	M	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
13	Z	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
All	All	3504/3614 (97%)	3204 (91%)	249 (7%)	51 (2%)	10	26

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	93	PRO
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
8	H	8	ILE
2	O	60	GLU
6	S	93	PRO
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	89	GLU

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Mol	Chain	Res	Type
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	10	ASN
1	N	9	SER
2	O	89	GLU
7	T	3	ALA
8	U	8	ILE
8	U	10	ASN
6	F	96	LEU
6	S	96	LEU
7	T	40	GLY
1	A	9	SER
7	G	54	ARG
1	N	91	ASP
3	P	38	ASN
10	W	15	ASP
1	A	91	ASP
1	A	369	ASP
3	C	38	ASN
10	J	15	ASP
2	O	59	GLN
2	O	202	SER
2	B	92	ASN
2	O	92	ASN
7	T	6	GLY
12	Y	28	PHE
7	G	6	GLY
1	A	174	PRO
8	H	47	GLY
7	T	49	PRO
8	U	47	GLY
1	N	296	GLY
2	O	159	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	415 (97%)	11 (3%)	46	75
1	N	426/426 (100%)	412 (97%)	14 (3%)	38	67
2	B	210/210 (100%)	192 (91%)	18 (9%)	10	24
2	O	210/210 (100%)	190 (90%)	20 (10%)	8	20
3	C	224/226 (99%)	213 (95%)	11 (5%)	25	52
3	P	224/226 (99%)	220 (98%)	4 (2%)	59	83
4	D	128/129 (99%)	123 (96%)	5 (4%)	32	61
4	Q	128/129 (99%)	123 (96%)	5 (4%)	32	61
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	67
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	57
6	F	81/81 (100%)	80 (99%)	1 (1%)	71	88
6	S	81/81 (100%)	74 (91%)	7 (9%)	10	24
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	22
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	22
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	35
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	35
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	35
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	65
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	81
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	81
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	50
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	50
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	50
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	50
13	M	37/38 (97%)	29 (78%)	8 (22%)	1	3
13	Z	37/38 (97%)	30 (81%)	7 (19%)	1	4
All	All	3040/3082 (99%)	2884 (95%)	156 (5%)	24	50

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	189	MET
1	A	238	PHE
1	A	241	PRO
1	A	336	PRO
1	A	369	ASP
1	A	377	PHE
1	A	444	PRO
1	A	503	HIS
2	B	3	TYR
2	B	16	ILE
2	B	21	LEU
2	B	43	SER
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	130	PRO
2	B	152	MET
2	B	167	SER
2	B	183	THR
2	B	185	MET
2	B	187	SER
2	B	199	ILE
3	C	13	PRO
3	C	17	PRO
3	C	39	SER
3	C	73	PRO
3	C	110	PRO
3	C	144	ILE
3	C	159	MET
3	C	179	SER
3	C	192	VAL
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
4	D	74	SER
4	D	108	PRO
4	D	121	LYS

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Mol	Chain	Res	Type
5	E	7	THR
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	27	ARG
8	H	29	CYS
8	H	60	TYR
8	H	62	SER
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
11	K	32	MET
11	K	54	ARG
12	L	15	VAL
12	L	26	THR
13	M	5	PRO
13	M	13	LYS
13	M	34	LEU
13	M	37	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	174	PRO
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	298	ASP
1	N	338	MET
1	N	356	ILE

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Mol	Chain	Res	Type
1	N	369	ASP
1	N	444	PRO
1	N	484	THR
1	N	498	CYS
2	O	3	TYR
2	O	16	ILE
2	O	43	SER
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	107	SER
2	O	110	TYR
2	O	115	ASP
2	O	156	SER
2	O	158	ASP
2	O	166	PRO
2	O	167	SER
2	O	183	THR
2	O	187	SER
2	O	223	SER
3	P	150	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	9	GLU
4	Q	10	ASP
4	Q	51	LEU
4	Q	110	THR
4	Q	121	LYS
5	R	5	HIS
5	R	80	GLU
5	R	87	GLN
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	50	PRO
6	S	53	THR
6	S	68	THR

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Mol	Chain	Res	Type
6	S	80	GLN
6	S	94	HIS
7	T	17	ARG
7	T	27	SER
7	T	33	LEU
7	T	35	SER
7	T	54	ARG
7	T	84	LYS
8	U	9	LYS
8	U	12	GLN
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	18	ARG
10	W	50	LEU
11	X	38	ILE
11	X	54	ARG
12	Y	11	ILE
12	Y	26	THR
13	Z	12	PRO
13	Z	13	LYS
13	Z	34	LEU
13	Z	37	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	151	HIS
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	91	ASN
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	76	GLN

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Mol	Chain	Res	Type
3	C	204	HIS
4	D	32	ASN
4	D	37	GLN
5	E	94	ASN
7	G	8	HIS
7	G	66	ASN
7	G	71	HIS
9	I	20	HIS
10	J	21	HIS
11	K	35	GLN
11	K	41	ASN
1	N	55	ASN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	491	ASN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	78	HIS
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
7	T	34	ASN
7	T	66	ASN
9	V	8	GLN
10	W	9	GLN
10	W	29	ASN
11	X	35	GLN
11	X	41	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	0.62	0	7,9,11	1.55	2 (28%)
7	TPO	G	11	7	8,10,11	1.86	3 (37%)	10,14,16	0.99	0
2	FME	B	1	2	8,9,10	0.74	0	7,9,11	1.61	2 (28%)
9	SAC	V	1	9	7,8,9	3.11	2 (28%)	8,9,11	3.11	5 (62%)
1	FME	N	1	1	8,9,10	0.98	0	7,9,11	0.86	0
7	TPO	T	11	7	8,10,11	1.91	4 (50%)	10,14,16	1.03	1 (10%)
9	SAC	I	1	9	7,8,9	2.82	2 (28%)	8,9,11	2.91	4 (50%)
1	FME	A	1	1	8,9,10	0.73	0	7,9,11	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
1	FME	N	1	1	-	5/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	5.58	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.42	1.35	1.23
9	V	1	SAC	OAC-C1A	5.38	1.35	1.23
9	I	1	SAC	CA-N	4.64	1.52	1.46
7	G	11	TPO	CB-CA	3.06	1.60	1.53
7	T	11	TPO	CG2-CB	2.79	1.58	1.51
7	G	11	TPO	CG2-CB	2.78	1.58	1.51
7	T	11	TPO	P-O1P	2.70	1.59	1.50
7	T	11	TPO	CB-CA	2.45	1.59	1.53
7	T	11	TPO	P-OG1	2.40	1.63	1.59
7	G	11	TPO	P-OG1	2.05	1.63	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-6.67	110.85	123.15
9	I	1	SAC	CA-N-C1A	-6.55	111.06	123.15
2	B	1	FME	CA-N-CN	-3.26	117.80	122.82
2	O	1	FME	C-CA-N	3.06	115.25	109.73
9	V	1	SAC	C2A-C1A-N	3.01	121.19	116.10
9	V	1	SAC	C-CA-N	-2.79	104.70	109.73
9	V	1	SAC	CB-CA-N	2.65	116.50	110.55
9	I	1	SAC	C-CA-N	-2.60	105.04	109.73
9	I	1	SAC	C2A-C1A-N	2.53	120.39	116.10
9	I	1	SAC	CB-CA-N	2.45	116.05	110.55
9	V	1	SAC	OAC-C1A-C2A	-2.44	117.52	122.06
2	O	1	FME	CA-N-CN	-2.35	119.21	122.82
2	B	1	FME	C-CA-N	2.17	113.65	109.73
7	T	11	TPO	O3P-P-OG1	2.04	115.11	105.99

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
2	B	1	FME	O1-CN-N-CA
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	O-C-CA-CB
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
1	A	1	FME	O1-CN-N-CA
2	B	1	FME	CB-CG-SD-CE
1	A	1	FME	CA-CB-CG-SD
7	T	11	TPO	CB-OG1-P-O2P
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CA-N-CN
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O3P
7	G	11	TPO	O-C-CA-CB
7	T	11	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	2	0
2	B	1	FME	2	0
1	N	1	FME	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 20 are monoatomic - leaving 44 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	TGL	N	1523	-	62,62,62	1.14	5 (8%)	65,65,65	1.43	9 (13%)
23	CHD	C	525	-	29,32,32	1.27	2 (6%)	48,51,51	2.19	15 (31%)
23	CHD	P	1271	-	29,32,32	1.33	6 (20%)	48,51,51	3.92	25 (52%)
26	CDL	P	1270	-	99,99,99	1.28	13 (13%)	105,111,111	1.05	8 (7%)
18	TGL	L	522	-	62,62,62	1.35	5 (8%)	65,65,65	1.74	13 (20%)
25	PEK	T	263	-	52,52,52	2.35	14 (26%)	55,57,57	1.38	8 (14%)
26	CDL	T	1269	-	99,99,99	1.44	15 (15%)	105,111,111	1.03	9 (8%)
25	PEK	P	1265	-	52,52,52	1.84	12 (23%)	55,57,57	1.09	5 (9%)
19	PGV	C	268	-	50,50,50	1.60	8 (16%)	53,56,56	0.91	2 (3%)
22	PSC	B	230	-	51,51,51	1.57	10 (19%)	57,59,59	1.09	3 (5%)
23	CHD	J	60	-	29,32,32	1.53	3 (10%)	48,51,51	3.83	25 (52%)
19	PGV	P	1267	-	50,50,50	1.10	4 (8%)	53,56,56	0.87	2 (3%)
25	PEK	C	264	-	52,52,52	2.05	12 (23%)	55,57,57	1.57	11 (20%)
25	PEK	G	1263	-	52,52,52	2.33	15 (28%)	55,57,57	1.38	7 (12%)
21	CUA	O	228	2	0,1,1	0.00	-	-	-	-
19	PGV	C	267	-	50,50,50	1.03	2 (4%)	53,56,56	1.07	6 (11%)
19	PGV	N	1266	-	50,50,50	1.23	6 (12%)	53,56,56	0.91	1 (1%)
22	PSC	O	1230	-	51,51,51	1.62	11 (21%)	57,59,59	1.06	4 (7%)
17	HEA	A	515	1	44,67,67	1.76	7 (15%)	37,103,103	1.66	9 (24%)
23	CHD	G	86	-	29,32,32	1.18	3 (10%)	48,51,51	2.66	21 (43%)
18	TGL	Y	1522	-	62,62,62	1.40	5 (8%)	65,65,65	1.68	10 (15%)
17	HEA	N	516	1	44,67,67	1.65	8 (18%)	37,103,103	1.49	5 (13%)
23	CHD	B	1086	-	29,32,32	0.88	0	48,51,51	2.51	20 (41%)
21	CUA	B	228	2	0,1,1	0.00	-	-	-	-
18	TGL	O	1521	-	62,62,62	1.03	5 (8%)	65,65,65	1.52	10 (15%)
24	DMU	P	1272	-	34,34,34	2.82	14 (41%)	45,45,45	3.72	19 (42%)
23	CHD	W	1060	-	29,32,32	1.82	5 (17%)	48,51,51	3.75	25 (52%)
17	HEA	A	516	1	44,67,67	1.52	8 (18%)	37,103,103	1.44	5 (13%)
24	DMU	Z	1526	-	34,34,34	3.34	9 (26%)	45,45,45	3.43	21 (46%)
23	CHD	C	271	-	29,32,32	1.28	4 (13%)	48,51,51	3.86	25 (52%)
18	TGL	A	521	-	62,62,62	0.97	3 (4%)	65,65,65	1.49	12 (18%)
25	PEK	C	265	-	52,52,52	1.89	12 (23%)	55,57,57	1.12	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	C	272	-	34,34,34	2.76	14 (41%)	45,45,45	3.92	18 (40%)
19	PGV	P	1268	-	50,50,50	1.61	9 (18%)	53,56,56	0.88	2 (3%)
17	HEA	N	515	1	44,67,67	2.26	10 (22%)	37,103,103	1.69	10 (27%)
25	PEK	T	1264	-	52,52,52	2.14	13 (25%)	55,57,57	1.55	10 (18%)
18	TGL	A	523	-	62,62,62	1.13	5 (8%)	65,65,65	1.41	11 (16%)
19	PGV	A	524	-	50,50,50	1.52	8 (16%)	53,56,56	1.10	5 (9%)
23	CHD	P	1525	-	29,32,32	1.49	5 (17%)	48,51,51	2.13	14 (29%)
26	CDL	C	270	-	99,99,99	1.22	13 (13%)	105,111,111	1.02	7 (6%)
19	PGV	A	525	-	50,50,50	1.12	5 (10%)	53,56,56	0.98	2 (3%)
19	PGV	N	1524	-	50,50,50	1.52	8 (16%)	53,56,56	1.06	5 (9%)
24	DMU	M	526	-	34,34,34	3.35	10 (29%)	45,45,45	3.52	21 (46%)
26	CDL	G	269	-	99,99,99	1.53	16 (16%)	105,111,111	1.02	7 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	TGL	N	1523	-	-	17/65/65/65	-
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
23	CHD	P	1271	-	5/5/12/12	6/7/74/74	0/4/4/4
26	CDL	P	1270	-	-	73/110/110/110	-
18	TGL	L	522	-	-	15/65/65/65	-
25	PEK	T	263	-	-	29/56/56/56	-
26	CDL	T	1269	-	-	66/110/110/110	-
25	PEK	P	1265	-	-	18/56/56/56	-
19	PGV	C	268	-	-	34/55/55/55	-
19	PGV	C	267	-	-	19/55/55/55	-
22	PSC	B	230	-	-	34/55/55/55	-
23	CHD	J	60	-	5/5/12/12	6/7/74/74	0/4/4/4
19	PGV	P	1267	-	-	19/55/55/55	-
25	PEK	C	264	-	-	21/56/56/56	-
25	PEK	G	1263	-	-	29/56/56/56	-
24	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	12/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSC	O	1230	-	-	34/55/55/55	-
17	HEA	A	515	1	3/3/7/16	7/24/76/76	-
23	CHD	G	86	-	-	0/7/74/74	0/4/4/4
18	TGL	Y	1522	-	-	17/65/65/65	-
17	HEA	N	516	1	3/3/7/16	2/24/76/76	-
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
18	TGL	O	1521	-	-	16/65/65/65	-
24	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
23	CHD	W	1060	-	5/5/12/12	6/7/74/74	0/4/4/4
17	HEA	A	516	1	3/3/7/16	2/24/76/76	-
25	PEK	T	1264	-	-	22/56/56/56	-
18	TGL	A	521	-	-	14/65/65/65	-
25	PEK	C	265	-	-	20/56/56/56	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
19	PGV	P	1268	-	-	35/55/55/55	-
17	HEA	N	515	1	3/3/7/16	7/24/76/76	-
23	CHD	C	271	-	5/5/12/12	6/7/74/74	0/4/4/4
18	TGL	A	523	-	-	17/65/65/65	-
19	PGV	A	524	-	-	34/55/55/55	-
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	CDL	C	270	-	-	70/110/110/110	-
19	PGV	A	525	-	-	11/55/55/55	-
19	PGV	N	1524	-	-	34/55/55/55	-
24	DMU	M	526	-	5/5/10/10	9/19/59/59	0/2/2/2
26	CDL	G	269	-	-	66/110/110/110	-

All (342) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C3B-C11	-11.25	1.44	1.52
24	Z	1526	DMU	O16-C6	-8.39	1.25	1.40
24	M	526	DMU	O16-C6	-8.14	1.26	1.40
17	A	515	HEA	C3B-C11	-7.88	1.46	1.52
24	M	526	DMU	O7-C3	-7.73	1.23	1.43
24	Z	1526	DMU	O5-C4	-7.47	1.26	1.44
24	Z	1526	DMU	O7-C3	-7.46	1.24	1.43
24	M	526	DMU	O1-C9	-7.28	1.26	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1526	DMU	O1-C9	-7.14	1.27	1.44
24	M	526	DMU	O5-C4	-7.14	1.27	1.44
18	Y	1522	TGL	OG2-CB1	6.99	1.54	1.34
25	G	1263	PEK	O03-C21	6.97	1.53	1.33
24	Z	1526	DMU	O16-C18	-6.82	1.24	1.43
24	M	526	DMU	O16-C18	-6.80	1.24	1.43
25	T	263	PEK	O03-C21	6.75	1.53	1.33
25	C	264	PEK	O01-C1	6.66	1.53	1.34
23	W	1060	CHD	C13-C17	6.52	1.66	1.55
17	N	516	HEA	C3B-C11	-6.48	1.47	1.52
23	J	60	CHD	C13-C17	6.25	1.66	1.55
25	T	1264	PEK	O01-C1	6.19	1.51	1.34
18	L	522	TGL	OG2-CB1	6.01	1.51	1.34
24	M	526	DMU	O7-C10	-5.91	1.25	1.41
24	Z	1526	DMU	O7-C10	-5.77	1.25	1.41
24	P	1272	DMU	O16-C18	-5.74	1.27	1.43
24	C	272	DMU	O16-C18	-5.60	1.27	1.43
25	T	1264	PEK	C15-C14	5.60	1.64	1.31
24	M	526	DMU	O1-C10	-5.54	1.27	1.41
19	N	1524	PGV	O03-C19	5.42	1.49	1.33
19	A	524	PGV	O03-C19	5.31	1.48	1.33
19	C	268	PGV	O01-C1	5.15	1.48	1.34
24	P	1272	DMU	C8-C9	5.15	1.63	1.53
25	G	1263	PEK	C6-C5	5.13	1.61	1.31
25	G	1263	PEK	C03-C02	5.11	1.66	1.50
25	C	264	PEK	C15-C14	5.10	1.61	1.31
24	Z	1526	DMU	O1-C10	-5.04	1.29	1.41
25	C	264	PEK	C12-C11	5.03	1.60	1.31
25	T	263	PEK	C15-C14	4.98	1.60	1.31
25	G	1263	PEK	C15-C14	4.95	1.60	1.31
25	T	263	PEK	C6-C5	4.89	1.60	1.31
25	T	263	PEK	C12-C11	4.88	1.60	1.31
26	G	269	CDL	OB6-CB5	4.88	1.48	1.34
24	P	1272	DMU	C8-C7	4.86	1.64	1.52
24	C	272	DMU	C8-C9	4.85	1.63	1.53
24	P	1272	DMU	C6-C1	4.85	1.66	1.52
24	P	1272	DMU	O7-C3	-4.85	1.31	1.43
24	C	272	DMU	C3-C4	4.84	1.65	1.52
24	C	272	DMU	C6-C1	4.82	1.66	1.52
25	T	263	PEK	C01-C02	4.81	1.65	1.50
22	O	1230	PSC	C10-C9	4.81	1.59	1.31
24	Z	1526	DMU	O5-C6	-4.80	1.29	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1265	PEK	C12-C11	4.78	1.59	1.31
25	C	265	PEK	C12-C11	4.74	1.59	1.31
19	C	268	PGV	C12-C11	4.74	1.59	1.31
25	T	1264	PEK	C6-C5	4.73	1.59	1.31
19	P	1268	PGV	O01-C1	4.73	1.47	1.34
25	G	1263	PEK	C12-C11	4.66	1.58	1.31
25	T	263	PEK	C03-C02	4.65	1.65	1.50
25	T	1264	PEK	C9-C8	4.64	1.58	1.31
19	P	1268	PGV	C12-C11	4.64	1.58	1.31
25	G	1263	PEK	C01-C02	4.60	1.64	1.50
24	P	1272	DMU	C3-C4	4.59	1.65	1.52
25	C	264	PEK	C6-C5	4.58	1.58	1.31
22	B	230	PSC	C10-C9	4.55	1.58	1.31
25	T	1264	PEK	C2-C1	4.53	1.64	1.50
25	C	265	PEK	C15-C14	4.50	1.57	1.31
26	G	269	CDL	OA6-CA5	4.48	1.46	1.34
24	P	1272	DMU	C7-C5	4.46	1.63	1.52
25	T	263	PEK	C9-C8	4.46	1.57	1.31
23	P	1525	CHD	C10-C9	-4.45	1.47	1.56
25	P	1265	PEK	C15-C14	4.44	1.57	1.31
19	A	524	PGV	C12-C11	4.41	1.57	1.31
25	G	1263	PEK	C9-C8	4.40	1.57	1.31
24	M	526	DMU	O5-C6	-4.36	1.30	1.41
25	P	1265	PEK	C9-C8	4.32	1.56	1.31
25	C	264	PEK	C9-C8	4.31	1.56	1.31
22	O	1230	PSC	C13-C12	4.31	1.56	1.31
19	N	1524	PGV	C12-C11	4.31	1.56	1.31
22	B	230	PSC	C13-C12	4.29	1.56	1.31
24	C	272	DMU	C7-C5	4.27	1.63	1.52
24	P	1272	DMU	C10-C5	4.27	1.64	1.52
25	T	1264	PEK	C12-C11	4.25	1.56	1.31
24	P	1272	DMU	O16-C6	-4.23	1.32	1.40
26	G	269	CDL	C51-CB5	4.18	1.62	1.50
24	C	272	DMU	C8-C7	4.17	1.62	1.52
26	T	1269	CDL	OB6-CB5	4.17	1.46	1.34
25	T	1264	PEK	P-O11	4.16	1.76	1.59
25	C	265	PEK	C9-C8	4.15	1.55	1.31
25	C	265	PEK	O01-C1	4.11	1.45	1.34
17	A	516	HEA	C3B-C11	-4.06	1.49	1.52
26	T	1269	CDL	C71-CB7	4.03	1.62	1.50
24	C	272	DMU	O5-C4	-4.03	1.34	1.44
18	Y	1522	TGL	CB2-CB1	3.99	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	525	CHD	C10-C9	-3.99	1.48	1.56
25	P	1265	PEK	C6-C5	3.99	1.54	1.31
26	T	1269	CDL	C51-CB5	3.96	1.62	1.50
18	L	522	TGL	CB2-CB1	3.95	1.62	1.50
26	G	269	CDL	C71-CB7	3.95	1.62	1.50
17	N	515	HEA	C3C-C2C	-3.95	1.34	1.40
19	N	1266	PGV	C12-C11	3.90	1.54	1.31
24	C	272	DMU	C2-C3	3.89	1.62	1.52
25	C	265	PEK	C6-C5	3.86	1.54	1.31
25	T	263	PEK	C22-C21	3.86	1.62	1.50
19	N	1266	PGV	O03-C19	3.83	1.44	1.33
19	A	525	PGV	C12-C11	3.79	1.53	1.31
25	C	265	PEK	P-O11	3.78	1.74	1.59
26	P	1270	CDL	OA8-CA7	3.78	1.44	1.33
26	P	1270	CDL	PB2-OB2	3.77	1.74	1.59
22	B	230	PSC	P-O12	3.76	1.74	1.59
23	P	1525	CHD	C13-C12	-3.75	1.48	1.54
17	A	515	HEA	C3A-CMA	-3.73	1.37	1.46
25	G	1263	PEK	P-O11	3.73	1.74	1.59
24	C	272	DMU	C10-C5	3.73	1.63	1.52
25	T	263	PEK	C2-C1	3.71	1.61	1.50
23	W	1060	CHD	C20-C17	3.71	1.60	1.54
25	C	265	PEK	O03-C21	3.71	1.44	1.33
17	N	515	HEA	C3A-C2A	-3.70	1.35	1.40
17	A	516	HEA	C4C-CHD	-3.69	1.30	1.41
24	C	272	DMU	O16-C6	-3.66	1.33	1.40
18	N	1523	TGL	OG1-CA1	3.66	1.44	1.33
24	C	272	DMU	O1-C9	-3.64	1.35	1.44
26	G	269	CDL	CB2-C1	3.63	1.64	1.51
23	G	86	CHD	C1-C10	-3.63	1.47	1.54
19	P	1267	PGV	C12-C11	3.62	1.52	1.31
26	C	270	CDL	OB8-CB7	3.61	1.43	1.33
26	G	269	CDL	CA6-CA4	3.59	1.61	1.50
26	G	269	CDL	CB6-CB4	3.58	1.61	1.50
25	P	1265	PEK	O03-C21	3.57	1.43	1.33
24	P	1272	DMU	C2-C1	3.57	1.61	1.52
19	C	267	PGV	C12-C11	3.57	1.52	1.31
19	P	1268	PGV	O03-C19	3.56	1.43	1.33
26	P	1270	CDL	OB8-CB7	3.56	1.43	1.33
25	T	263	PEK	P-O11	3.56	1.73	1.59
26	C	270	CDL	PB2-OB2	3.56	1.73	1.59
24	C	272	DMU	O7-C3	-3.55	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	1230	PSC	C2-C1	3.54	1.61	1.50
19	A	524	PGV	C20-C19	3.51	1.61	1.50
18	A	523	TGL	CB2-CB1	3.47	1.60	1.50
17	N	515	HEA	C3A-CMA	-3.45	1.38	1.46
18	O	1521	TGL	OG2-CB1	3.43	1.44	1.34
25	T	1264	PEK	C22-C21	3.42	1.60	1.50
25	P	1265	PEK	C22-C21	3.41	1.60	1.50
22	O	1230	PSC	P-O12	3.41	1.73	1.59
17	N	516	HEA	C4C-CHD	-3.40	1.31	1.41
19	C	268	PGV	O03-C19	3.39	1.43	1.33
17	A	516	HEA	C3C-C2C	-3.38	1.35	1.40
26	C	270	CDL	C71-CB7	3.38	1.60	1.50
25	C	265	PEK	P-O12	3.38	1.73	1.59
17	N	515	HEA	C3B-C2B	-3.37	1.30	1.41
26	T	1269	CDL	CB6-CB4	3.34	1.60	1.50
26	T	1269	CDL	CB2-C1	3.34	1.63	1.51
25	C	265	PEK	C22-C21	3.33	1.60	1.50
25	T	263	PEK	O01-C1	3.33	1.43	1.34
19	C	268	PGV	C2-C1	3.33	1.60	1.50
19	N	1524	PGV	C20-C19	3.30	1.60	1.50
25	G	1263	PEK	C22-C21	3.30	1.60	1.50
18	A	523	TGL	OG2-CB1	3.25	1.43	1.34
25	P	1265	PEK	P-O11	3.24	1.72	1.59
25	T	1264	PEK	P-O12	3.22	1.72	1.59
18	A	521	TGL	CG3-CG2	3.21	1.60	1.50
24	C	272	DMU	C2-C1	3.20	1.60	1.52
19	N	1266	PGV	C2-C1	3.20	1.60	1.50
23	C	271	CHD	C13-C17	3.19	1.61	1.55
26	T	1269	CDL	OA6-CA5	3.19	1.43	1.34
24	P	1272	DMU	O5-C4	-3.18	1.36	1.44
26	P	1270	CDL	C71-CB7	3.15	1.59	1.50
25	C	264	PEK	P-O12	3.15	1.72	1.59
19	P	1268	PGV	C2-C1	3.15	1.59	1.50
26	G	269	CDL	OA8-CA7	3.12	1.42	1.33
18	L	522	TGL	CC2-CC1	3.11	1.59	1.50
26	P	1270	CDL	OB6-CB5	3.09	1.43	1.34
26	T	1269	CDL	OB8-CB7	3.06	1.42	1.33
24	P	1272	DMU	C2-C3	3.05	1.60	1.52
22	B	230	PSC	O01-C1	3.04	1.42	1.34
25	P	1265	PEK	O01-C1	3.04	1.42	1.34
25	G	1263	PEK	P-O12	3.03	1.71	1.59
19	P	1267	PGV	O03-C19	3.03	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	523	TGL	OG1-CA1	3.02	1.42	1.33
25	C	264	PEK	O03-C21	3.01	1.42	1.33
26	T	1269	CDL	CA6-CA4	3.01	1.59	1.50
18	Y	1522	TGL	OG1-CA1	3.00	1.42	1.33
26	C	270	CDL	CA3-CA4	2.97	1.59	1.50
17	A	516	HEA	C21-C22	2.97	1.60	1.50
18	N	1523	TGL	CA2-CA1	2.97	1.59	1.50
19	N	1524	PGV	P-O11	2.96	1.71	1.59
18	N	1523	TGL	OG3-CC1	2.96	1.42	1.33
23	J	60	CHD	C20-C17	2.93	1.59	1.54
18	N	1523	TGL	CB2-CB1	2.93	1.59	1.50
17	A	515	HEA	C3A-C2A	-2.92	1.36	1.40
17	A	516	HEA	C1B-CHB	-2.92	1.32	1.41
22	O	1230	PSC	O01-C1	2.91	1.42	1.34
25	P	1265	PEK	P-O12	2.90	1.71	1.59
26	T	1269	CDL	C11-CA5	2.89	1.59	1.50
25	G	1263	PEK	O03-C01	2.87	1.51	1.45
23	W	1060	CHD	C13-C12	2.86	1.59	1.54
23	P	1271	CHD	C13-C14	2.84	1.60	1.55
26	P	1270	CDL	C11-CA5	2.84	1.59	1.50
26	C	270	CDL	CA6-CA4	2.84	1.59	1.50
26	T	1269	CDL	CB3-CB4	2.82	1.59	1.50
25	G	1263	PEK	C2-C1	2.82	1.59	1.50
19	A	525	PGV	C03-C02	2.80	1.59	1.50
19	A	525	PGV	O01-C1	2.79	1.42	1.34
19	C	267	PGV	C01-C02	2.79	1.59	1.50
19	P	1268	PGV	C04-C05	2.79	1.61	1.51
19	A	525	PGV	O03-C19	2.78	1.41	1.33
18	A	523	TGL	OG3-CC1	2.77	1.41	1.33
22	B	230	PSC	C2-C1	2.76	1.58	1.50
17	A	515	HEA	C3C-C2C	-2.75	1.36	1.40
26	C	270	CDL	C31-CA7	2.75	1.58	1.50
25	T	263	PEK	O03-C01	2.75	1.51	1.45
22	B	230	PSC	C05-C04	2.74	1.59	1.51
25	T	263	PEK	P-O12	2.74	1.70	1.59
22	O	1230	PSC	O03-C19	2.73	1.41	1.33
19	A	524	PGV	P-O12	2.73	1.70	1.59
23	C	525	CHD	C13-C12	-2.73	1.50	1.54
18	O	1521	TGL	CG3-CG2	2.73	1.59	1.50
19	C	268	PGV	P-O11	2.71	1.70	1.59
17	A	515	HEA	C3B-C2B	-2.70	1.32	1.41
26	G	269	CDL	CB3-CB4	2.68	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	1522	TGL	CG1-CG2	2.68	1.58	1.50
19	N	1524	PGV	O01-C1	2.66	1.41	1.34
25	C	264	PEK	C2-C1	2.66	1.58	1.50
17	N	515	HEA	C20-C19	2.65	1.56	1.51
17	A	516	HEA	C3A-C2A	-2.65	1.36	1.40
23	P	1271	CHD	C13-C17	2.64	1.60	1.55
19	P	1268	PGV	C20-C19	2.64	1.58	1.50
19	C	268	PGV	P-O12	2.64	1.70	1.59
19	P	1268	PGV	P-O12	2.64	1.70	1.59
18	O	1521	TGL	OG3-CC1	2.63	1.41	1.33
25	P	1265	PEK	C03-C02	2.61	1.58	1.50
23	C	271	CHD	C13-C14	2.58	1.59	1.55
25	P	1265	PEK	C01-C02	2.57	1.58	1.50
17	N	516	HEA	C21-C22	2.56	1.58	1.50
18	L	522	TGL	CG1-CG2	2.56	1.58	1.50
18	O	1521	TGL	CA2-CA1	2.54	1.58	1.50
23	G	86	CHD	C8-C9	2.53	1.58	1.53
25	C	264	PEK	P-O11	2.53	1.69	1.59
18	A	521	TGL	OG2-CB1	2.51	1.41	1.34
25	G	1263	PEK	O01-C1	2.49	1.41	1.34
19	A	524	PGV	P-O11	2.49	1.69	1.59
26	C	270	CDL	OA8-CA7	2.48	1.40	1.33
22	O	1230	PSC	P-O11	2.48	1.69	1.59
23	P	1525	CHD	C10-C5	-2.48	1.51	1.55
22	B	230	PSC	O03-C19	2.48	1.40	1.33
17	N	516	HEA	C3C-C2C	-2.47	1.36	1.40
26	P	1270	CDL	CA3-CA4	2.47	1.58	1.50
17	N	516	HEA	C3B-C2B	-2.46	1.33	1.41
26	P	1270	CDL	C31-CA7	2.46	1.57	1.50
26	G	269	CDL	C31-CA7	2.46	1.57	1.50
19	N	1524	PGV	C03-C02	2.44	1.58	1.50
26	C	270	CDL	OB6-CB5	2.44	1.41	1.34
23	W	1060	CHD	C8-C7	2.44	1.57	1.53
19	N	1266	PGV	C20-C19	2.44	1.57	1.50
26	G	269	CDL	OB8-CB7	2.43	1.40	1.33
23	C	271	CHD	C13-C12	2.43	1.58	1.54
23	P	1271	CHD	C10-C5	2.43	1.59	1.55
19	C	268	PGV	C04-C05	2.42	1.59	1.51
17	N	516	HEA	C22-C23	2.41	1.39	1.32
19	P	1268	PGV	C06-C05	2.41	1.61	1.51
25	C	264	PEK	C22-C21	2.41	1.57	1.50
24	P	1272	DMU	O1-C9	-2.40	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	PA1-OA5	2.40	1.69	1.59
22	O	1230	PSC	C01-C02	2.40	1.58	1.50
23	P	1525	CHD	C18-C13	-2.40	1.50	1.54
18	L	522	TGL	OG1-CA1	2.40	1.40	1.33
17	A	516	HEA	C3A-CMA	-2.40	1.40	1.46
19	A	524	PGV	O01-C1	2.39	1.41	1.34
26	C	270	CDL	C11-CA5	2.39	1.57	1.50
23	P	1271	CHD	C8-C9	2.39	1.58	1.53
17	N	515	HEA	C1D-C2D	2.38	1.48	1.42
22	B	230	PSC	C03-C02	2.38	1.58	1.50
25	C	265	PEK	C03-C02	2.38	1.58	1.50
26	P	1270	CDL	PB2-OB5	2.36	1.68	1.59
18	A	521	TGL	CA2-CA1	2.36	1.57	1.50
26	T	1269	CDL	PA1-OA5	2.36	1.68	1.59
25	T	1264	PEK	C16-C15	2.36	1.63	1.50
19	N	1266	PGV	C01-C02	2.35	1.57	1.50
18	Y	1522	TGL	CC2-CC1	2.35	1.57	1.50
17	N	515	HEA	C4D-CHA	-2.35	1.34	1.41
25	C	265	PEK	C2-C1	2.35	1.57	1.50
19	A	524	PGV	C03-C02	2.34	1.57	1.50
26	P	1270	CDL	CA6-CA4	2.34	1.57	1.50
17	N	516	HEA	C3A-CMA	-2.34	1.40	1.46
26	P	1270	CDL	OA6-CA5	2.34	1.40	1.34
26	P	1270	CDL	CB2-C1	2.34	1.59	1.51
22	B	230	PSC	P-O11	2.31	1.68	1.59
26	T	1269	CDL	PA1-OA2	2.31	1.68	1.59
26	G	269	CDL	PA1-OA2	2.31	1.68	1.59
26	G	269	CDL	C11-CA5	2.30	1.57	1.50
24	C	272	DMU	O7-C10	-2.29	1.35	1.41
24	P	1272	DMU	O7-C10	-2.28	1.35	1.41
26	C	270	CDL	OA6-CA5	2.28	1.40	1.34
23	G	86	CHD	C10-C5	-2.28	1.51	1.55
19	P	1268	PGV	P-O11	2.27	1.68	1.59
23	P	1271	CHD	C13-C12	2.27	1.58	1.54
17	A	515	HEA	C1B-CHB	-2.27	1.34	1.41
22	O	1230	PSC	C05-C04	2.25	1.58	1.51
26	T	1269	CDL	OA8-CA7	2.25	1.39	1.33
19	N	1524	PGV	P-O12	2.25	1.68	1.59
19	N	1266	PGV	C03-C02	2.25	1.57	1.50
23	W	1060	CHD	C8-C14	2.25	1.58	1.53
25	T	1264	PEK	O03-C21	2.25	1.39	1.33
19	A	524	PGV	C06-C05	2.24	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	1269	CDL	C85-C84	2.23	1.64	1.51
25	C	264	PEK	P-O14	2.23	1.58	1.50
18	A	523	TGL	CA2-CA1	2.22	1.57	1.50
17	A	515	HEA	C1C-CHC	-2.22	1.34	1.41
23	J	60	CHD	C8-C7	2.21	1.57	1.53
22	B	230	PSC	C01-C02	2.21	1.57	1.50
19	P	1267	PGV	C20-C19	2.20	1.57	1.50
24	M	526	DMU	C8-C9	2.20	1.57	1.53
19	A	525	PGV	C20-C19	2.20	1.57	1.50
17	N	516	HEA	C3A-C2A	-2.18	1.37	1.40
26	P	1270	CDL	PA1-OA5	2.18	1.68	1.59
17	N	515	HEA	C16-C15	2.18	1.55	1.51
19	C	268	PGV	C06-C05	2.18	1.60	1.51
25	G	1263	PEK	C23-C22	2.18	1.60	1.52
19	P	1267	PGV	C01-C02	2.16	1.57	1.50
26	G	269	CDL	PB2-OB2	2.15	1.68	1.59
26	C	270	CDL	PB2-OB5	2.15	1.68	1.59
25	T	1264	PEK	C01-C02	2.14	1.57	1.50
17	N	515	HEA	C1B-CHB	-2.13	1.35	1.41
22	O	1230	PSC	C20-C19	2.13	1.56	1.50
25	C	265	PEK	C01-C02	2.12	1.57	1.50
25	G	1263	PEK	C4-C5	2.09	1.61	1.50
18	O	1521	TGL	CC2-CC1	2.08	1.56	1.50
26	T	1269	CDL	PB2-OB2	2.06	1.67	1.59
25	T	1264	PEK	C4-C5	2.05	1.61	1.50
17	A	516	HEA	C22-C23	2.05	1.38	1.32
25	T	263	PEK	C23-C22	2.05	1.59	1.52
22	O	1230	PSC	C03-C02	2.04	1.57	1.50
18	N	1523	TGL	OG2-CB1	2.04	1.40	1.34
25	P	1265	PEK	C2-C1	2.04	1.56	1.50
24	Z	1526	DMU	C8-C7	2.03	1.57	1.52
26	C	270	CDL	CB2-C1	2.03	1.58	1.51
23	P	1525	CHD	C13-C17	-2.03	1.52	1.55
25	C	264	PEK	C18-C17	2.02	1.63	1.51
26	C	270	CDL	PA1-OA5	2.02	1.67	1.59
19	N	1524	PGV	C06-C05	2.02	1.60	1.51
23	C	271	CHD	C8-C14	2.01	1.57	1.53
23	P	1271	CHD	C8-C7	2.01	1.56	1.53
26	G	269	CDL	C85-C84	2.00	1.62	1.51
24	M	526	DMU	C8-C7	2.00	1.57	1.52

All (452) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C10-C9-C8	11.85	124.55	111.82
23	C	271	CHD	C10-C9-C8	11.73	124.42	111.82
24	P	1272	DMU	O16-C6-C1	11.15	125.71	108.30
23	J	60	CHD	C13-C17-C20	10.03	131.46	119.50
23	C	271	CHD	C17-C13-C14	9.48	109.65	100.09
24	C	272	DMU	O16-C6-C1	9.28	122.80	108.30
23	W	1060	CHD	C13-C17-C20	9.22	130.50	119.50
23	J	60	CHD	C17-C13-C14	9.17	109.34	100.09
23	P	1271	CHD	C17-C13-C14	9.01	109.18	100.09
24	Z	1526	DMU	O1-C9-C11	8.91	128.59	106.44
24	M	526	DMU	O1-C9-C11	8.87	128.50	106.44
24	C	272	DMU	C1-C2-C3	8.72	129.60	109.68
23	W	1060	CHD	C17-C13-C14	8.48	108.65	100.09
24	P	1272	DMU	O1-C9-C11	8.23	126.89	106.44
23	J	60	CHD	C11-C12-C13	8.10	119.56	111.24
24	Z	1526	DMU	O5-C4-C3	7.82	126.24	109.75
23	W	1060	CHD	C10-C9-C8	7.79	120.18	111.82
23	C	271	CHD	C19-C10-C9	-7.73	100.53	111.18
24	C	272	DMU	O1-C9-C11	7.63	125.40	106.44
23	P	1271	CHD	C19-C10-C9	-7.58	100.74	111.18
23	P	1271	CHD	C17-C13-C12	-7.46	110.86	117.67
24	C	272	DMU	C18-O16-C6	7.40	126.12	113.84
24	C	272	DMU	O5-C4-C3	7.39	125.34	109.75
23	W	1060	CHD	C11-C12-C13	7.30	118.74	111.24
23	J	60	CHD	C10-C9-C8	7.28	119.64	111.82
23	P	1271	CHD	C9-C8-C7	7.23	120.52	111.88
23	G	86	CHD	C17-C13-C14	7.10	107.25	100.09
24	C	272	DMU	C6-O5-C4	6.98	127.39	113.69
24	M	526	DMU	O5-C4-C3	6.97	124.45	109.75
23	J	60	CHD	C6-C5-C10	6.96	120.05	112.66
24	P	1272	DMU	O5-C4-C3	6.95	124.41	109.75
23	W	1060	CHD	C6-C5-C10	6.91	120.00	112.66
23	J	60	CHD	C18-C13-C14	-6.77	100.61	111.21
23	C	271	CHD	C9-C8-C7	6.76	119.96	111.88
24	M	526	DMU	O5-C6-O16	6.71	125.87	109.97
24	P	1272	DMU	C6-O5-C4	6.69	126.82	113.69
24	M	526	DMU	C6-O5-C4	6.68	126.80	113.69
24	M	526	DMU	C7-C8-C9	6.68	122.15	110.24
23	C	271	CHD	C19-C10-C1	-6.66	97.53	108.26
24	C	272	DMU	O7-C3-C4	6.63	127.61	109.45
23	W	1060	CHD	C18-C13-C14	-6.61	100.86	111.21
24	M	526	DMU	O5-C4-C57	6.59	122.83	106.44
23	W	1060	CHD	C4-C3-C2	6.54	118.36	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	C7-C8-C9	6.49	121.82	110.24
23	P	1525	CHD	C13-C17-C20	6.46	127.21	119.50
23	J	60	CHD	C4-C3-C2	6.45	118.26	110.55
24	P	1272	DMU	O7-C3-C4	6.42	127.03	109.45
23	W	1060	CHD	C5-C6-C7	6.41	121.54	114.46
23	G	86	CHD	C9-C8-C7	-6.41	104.21	111.88
23	B	1086	CHD	C17-C13-C14	6.33	106.48	100.09
24	C	272	DMU	O7-C3-C2	6.27	123.96	107.28
23	P	1271	CHD	C1-C10-C5	6.23	116.99	107.77
24	Z	1526	DMU	O5-C6-O16	6.19	124.63	109.97
23	C	271	CHD	C17-C13-C12	-6.19	112.02	117.67
23	J	60	CHD	C5-C6-C7	6.11	121.20	114.46
23	C	271	CHD	C1-C10-C5	6.10	116.79	107.77
24	C	272	DMU	O5-C6-C1	6.04	123.13	110.35
24	P	1272	DMU	O5-C4-C57	6.02	121.40	106.44
23	P	1271	CHD	C19-C10-C1	-6.02	98.57	108.26
23	P	1271	CHD	C6-C5-C10	5.99	119.02	112.66
24	Z	1526	DMU	C6-O5-C4	5.97	125.41	113.69
24	Z	1526	DMU	O5-C4-C57	5.95	121.23	106.44
23	B	1086	CHD	C9-C8-C7	-5.89	104.83	111.88
24	C	272	DMU	O1-C9-C8	5.88	120.36	109.69
24	P	1272	DMU	C1-C2-C3	5.82	122.96	109.68
24	M	526	DMU	O7-C3-C2	5.71	122.47	107.28
23	B	1086	CHD	C16-C17-C13	-5.67	97.99	103.55
23	C	271	CHD	C6-C5-C10	5.61	118.61	112.66
23	C	525	CHD	C13-C17-C20	5.60	126.18	119.50
24	C	272	DMU	O7-C10-C5	5.53	122.42	108.10
23	J	60	CHD	C9-C8-C7	5.51	118.47	111.88
24	Z	1526	DMU	O5-C6-C1	5.49	121.97	110.35
23	G	86	CHD	C16-C17-C13	-5.43	98.23	103.55
24	P	1272	DMU	O5-C6-C1	5.39	121.77	110.35
23	W	1060	CHD	C9-C8-C7	5.27	118.18	111.88
23	C	525	CHD	C14-C8-C9	-5.21	102.55	109.71
18	L	522	TGL	C12-C11-C10	-5.20	88.04	114.42
24	C	272	DMU	O5-C4-C57	5.19	119.34	106.44
23	P	1271	CHD	C15-C14-C8	-5.16	111.12	118.33
24	M	526	DMU	O5-C6-C1	5.14	121.23	110.35
23	J	60	CHD	C15-C14-C8	-5.12	111.18	118.33
23	W	1060	CHD	C1-C10-C5	5.10	115.31	107.77
23	P	1271	CHD	C4-C3-C2	5.09	116.63	110.55
23	C	271	CHD	C4-C3-C2	5.05	116.59	110.55
24	P	1272	DMU	O1-C9-C8	5.03	118.84	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	1522	TGL	C12-C11-C10	-4.99	89.08	114.42
18	O	1521	TGL	CG2-OG2-CB1	4.99	130.07	117.79
23	J	60	CHD	C1-C10-C5	4.97	115.12	107.77
24	P	1272	DMU	C18-O16-C6	4.97	122.07	113.84
24	Z	1526	DMU	O7-C3-C2	4.96	120.48	107.28
24	C	272	DMU	C8-C7-C5	4.96	119.48	110.82
24	P	1272	DMU	O7-C3-C2	4.94	120.42	107.28
23	G	86	CHD	C15-C14-C13	-4.84	98.81	103.55
24	M	526	DMU	C10-C5-C7	4.83	120.05	110.00
23	C	525	CHD	C2-C1-C10	4.82	121.05	112.78
23	W	1060	CHD	C15-C14-C8	-4.71	111.75	118.33
23	P	1271	CHD	C14-C13-C12	4.70	111.78	107.40
24	Z	1526	DMU	O7-C3-C4	4.69	122.31	109.45
23	G	86	CHD	C10-C9-C8	4.65	116.81	111.82
24	M	526	DMU	O7-C10-C5	4.64	120.11	108.10
18	A	521	TGL	CG2-OG2-CB1	4.61	129.14	117.79
18	A	521	TGL	CG1-OG1-CA1	-4.54	100.30	117.12
23	C	271	CHD	C15-C14-C8	-4.53	112.00	118.33
23	P	1271	CHD	C5-C6-C7	4.51	119.44	114.46
24	M	526	DMU	O1-C9-C8	4.51	117.88	109.69
23	C	271	CHD	C14-C8-C7	4.49	117.76	111.81
23	P	1525	CHD	C2-C1-C10	4.48	120.46	112.78
18	L	522	TGL	CB9-CB8-CB7	-4.44	91.88	114.42
24	Z	1526	DMU	C18-O16-C6	4.44	121.20	113.84
24	Z	1526	DMU	O1-C9-C8	4.43	117.73	109.69
24	M	526	DMU	O7-C3-C4	4.41	121.54	109.45
18	Y	1522	TGL	CB9-CB8-CB7	-4.39	92.13	114.42
23	C	271	CHD	C4-C5-C10	4.39	117.32	112.66
18	O	1521	TGL	CG1-OG1-CA1	-4.37	100.94	117.12
24	Z	1526	DMU	C10-C5-C7	4.36	119.07	110.00
23	P	1271	CHD	C14-C8-C7	4.25	117.45	111.81
23	C	525	CHD	O12-C12-C11	4.25	117.78	109.12
17	N	516	HEA	C3C-C4C-NC	4.24	114.69	109.21
25	T	263	PEK	C02-O01-C1	4.21	128.16	117.79
18	L	522	TGL	CG2-OG2-CB1	4.16	128.04	117.79
25	T	263	PEK	P-O11-C03	4.15	146.01	121.68
25	G	1263	PEK	P-O11-C03	4.12	145.85	121.68
18	L	522	TGL	C15-CC9-CC8	4.12	135.33	114.42
19	A	525	PGV	O01-C1-C2	-4.11	102.63	111.50
17	N	515	HEA	C26-C15-C16	4.11	122.19	115.27
23	P	1525	CHD	C14-C8-C9	-4.10	104.08	109.71
23	C	271	CHD	C5-C6-C7	4.10	118.98	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	264	PEK	C2-C3-C4	-4.09	105.94	113.23
23	W	1060	CHD	C6-C5-C4	4.08	115.89	111.19
24	M	526	DMU	C10-O7-C3	4.06	128.02	117.96
18	Y	1522	TGL	C15-CC9-CC8	4.04	134.96	114.42
24	M	526	DMU	C1-C2-C3	4.03	118.88	109.68
24	P	1272	DMU	C8-C7-C5	4.01	117.83	110.82
23	B	1086	CHD	C5-C4-C3	4.01	118.64	112.76
17	N	516	HEA	C20-C21-C22	4.00	125.03	111.88
25	G	1263	PEK	O03-C01-C02	3.99	120.04	108.43
25	T	263	PEK	O03-C01-C02	3.98	120.01	108.43
24	Z	1526	DMU	C1-C2-C3	3.96	118.72	109.68
25	G	1263	PEK	C02-O01-C1	3.95	127.53	117.79
23	J	60	CHD	C13-C14-C8	3.94	119.77	114.74
23	B	1086	CHD	C15-C14-C13	-3.93	99.70	103.55
24	Z	1526	DMU	O7-C10-C5	3.93	118.28	108.10
18	Y	1522	TGL	C16-C15-CC9	3.92	134.31	114.42
24	P	1272	DMU	O7-C10-O1	3.88	121.52	110.67
23	W	1060	CHD	C13-C14-C8	3.88	119.70	114.74
23	G	86	CHD	C1-C2-C3	3.88	115.45	110.47
18	L	522	TGL	CC3-CC2-CC1	3.88	127.71	113.62
23	G	86	CHD	C5-C4-C3	3.87	118.44	112.76
23	J	60	CHD	C2-C1-C10	3.87	119.42	112.78
23	C	271	CHD	C1-C10-C9	3.86	117.43	111.35
24	P	1272	DMU	O1-C10-C5	3.86	118.52	110.35
23	P	1525	CHD	C15-C14-C8	-3.85	112.94	118.33
23	B	1086	CHD	C15-C14-C8	-3.84	112.96	118.33
23	C	525	CHD	C15-C14-C8	-3.83	112.98	118.33
23	W	1060	CHD	C2-C1-C10	3.83	119.34	112.78
23	P	1525	CHD	C1-C10-C5	3.81	113.40	107.77
24	C	272	DMU	C10-O1-C9	3.80	121.15	113.69
23	P	1271	CHD	C4-C5-C10	3.80	116.69	112.66
18	L	522	TGL	C16-C15-CC9	3.78	133.62	114.42
24	P	1272	DMU	O7-C10-C5	3.76	117.85	108.10
23	C	525	CHD	C1-C10-C5	3.76	113.33	107.77
23	P	1271	CHD	C1-C10-C9	3.75	117.24	111.35
18	L	522	TGL	C11-C10-CB9	3.74	133.40	114.42
18	A	523	TGL	CG3-OG3-CC1	3.74	130.96	117.12
23	C	271	CHD	C18-C13-C12	-3.74	105.26	109.07
23	P	1525	CHD	C1-C2-C3	3.72	115.24	110.47
23	J	60	CHD	C1-C2-C3	3.71	115.23	110.47
23	G	86	CHD	C15-C14-C8	-3.71	113.15	118.33
17	N	515	HEA	C27-C19-C18	-3.71	114.17	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	264	PEK	C01-O03-C21	-3.68	103.50	117.12
23	B	1086	CHD	C11-C12-C13	-3.65	107.49	111.24
23	B	1086	CHD	C10-C9-C8	3.64	115.73	111.82
25	T	1264	PEK	C02-O01-C1	-3.62	108.88	117.79
17	A	516	HEA	C20-C21-C22	3.61	123.75	111.88
18	Y	1522	TGL	CC3-CC2-CC1	3.61	126.75	113.62
17	A	515	HEA	C27-C19-C18	-3.58	114.50	123.68
23	C	271	CHD	C14-C13-C12	3.55	110.71	107.40
18	N	1523	TGL	CG3-OG3-CC1	3.54	130.24	117.12
23	B	1086	CHD	C9-C11-C12	3.54	118.98	114.30
23	P	1525	CHD	C6-C5-C10	3.53	116.41	112.66
18	Y	1522	TGL	C11-C10-CB9	3.53	132.32	114.42
18	N	1523	TGL	OG2-CB1-CB2	-3.52	103.91	111.50
22	B	230	PSC	C01-O03-C19	-3.52	104.09	117.12
23	G	86	CHD	O3-C3-C4	-3.52	102.85	109.85
17	A	516	HEA	C3C-C4C-NC	3.48	113.71	109.21
26	C	270	CDL	PA1-OA5-CA3	3.48	142.09	121.68
24	M	526	DMU	C18-O16-C6	3.44	119.55	113.84
17	N	516	HEA	C20-C19-C18	-3.42	114.19	121.12
26	P	1270	CDL	CB6-OB8-CB7	-3.42	104.47	117.12
18	Y	1522	TGL	CG2-OG2-CB1	3.42	126.20	117.79
23	B	1086	CHD	C1-C2-C3	3.41	114.84	110.47
19	N	1524	PGV	O01-C02-C03	3.40	120.72	108.40
24	C	272	DMU	O7-C10-O1	3.40	120.16	110.67
23	W	1060	CHD	C1-C2-C3	3.39	114.81	110.47
23	W	1060	CHD	C9-C11-C12	3.37	118.76	114.30
23	P	1271	CHD	C18-C13-C12	-3.37	105.64	109.07
25	T	1264	PEK	C01-O03-C21	-3.36	104.69	117.12
23	G	86	CHD	C5-C6-C7	3.35	118.16	114.46
18	N	1523	TGL	CB3-CB2-CB1	3.35	125.81	113.62
18	A	523	TGL	CB3-CB2-CB1	3.35	125.80	113.62
24	P	1272	DMU	C10-O1-C9	3.34	120.25	113.69
23	G	86	CHD	C1-C10-C5	3.34	112.71	107.77
19	A	524	PGV	C3-C2-C1	-3.33	101.52	113.62
26	P	1270	CDL	PA1-OA5-CA3	3.31	141.11	121.68
23	J	60	CHD	C6-C5-C4	3.31	115.00	111.19
23	P	1271	CHD	C5-C4-C3	3.30	117.60	112.76
17	A	515	HEA	C27-C19-C20	3.28	120.80	115.27
18	N	1523	TGL	CG1-OG1-CA1	-3.28	104.97	117.12
25	C	264	PEK	P-O12-C04	-3.28	105.45	121.59
23	B	1086	CHD	C14-C8-C9	-3.26	105.24	109.71
17	A	515	HEA	C26-C15-C16	3.26	120.75	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	1523	TGL	OG2-CG2-CG3	3.23	120.10	108.40
23	B	1086	CHD	C1-C10-C5	3.22	112.53	107.77
23	C	525	CHD	C5-C6-C7	3.21	118.00	114.46
19	A	524	PGV	O01-C02-C03	3.20	119.99	108.40
23	C	525	CHD	C1-C2-C3	3.18	114.55	110.47
25	C	265	PEK	P-O11-C03	3.17	140.28	121.68
25	T	1264	PEK	P-O12-C04	-3.16	106.03	121.59
23	J	60	CHD	C16-C15-C14	3.15	111.38	105.13
23	W	1060	CHD	C16-C15-C14	3.15	111.38	105.13
23	P	1525	CHD	C5-C6-C7	3.15	117.93	114.46
23	G	86	CHD	C19-C10-C5	-3.14	105.03	110.36
23	C	271	CHD	C5-C4-C3	3.13	117.35	112.76
24	Z	1526	DMU	O16-C6-C1	3.13	113.19	108.30
17	A	516	HEA	CMC-C2C-C1C	-3.12	123.67	128.46
26	C	270	CDL	CB6-OB8-CB7	-3.09	105.67	117.12
22	B	230	PSC	P-O12-C04	3.09	136.81	121.59
23	J	60	CHD	C15-C16-C17	3.08	111.24	105.13
24	P	1272	DMU	C7-C8-C9	3.08	115.73	110.24
19	N	1266	PGV	O01-C1-C2	-3.08	104.87	111.50
25	T	1264	PEK	C2-C3-C4	-3.07	107.75	113.23
25	T	1264	PEK	C23-C22-C21	-3.05	102.53	113.62
24	Z	1526	DMU	O7-C10-O1	3.05	119.18	110.67
23	W	1060	CHD	C19-C10-C5	-3.04	105.20	110.36
23	W	1060	CHD	C15-C16-C17	3.03	111.14	105.13
23	C	271	CHD	C16-C15-C14	3.03	111.13	105.13
25	T	263	PEK	C2-C3-C4	3.03	118.62	113.23
25	C	265	PEK	C11-C10-C9	3.03	126.93	112.02
23	P	1525	CHD	C11-C9-C10	-3.02	110.61	113.73
23	W	1060	CHD	C18-C13-C12	-3.02	105.99	109.07
26	T	1269	CDL	C22-C21-C20	3.02	129.77	114.42
24	Z	1526	DMU	O1-C10-C5	3.02	116.74	110.35
24	M	526	DMU	O1-C10-C5	3.02	116.73	110.35
25	C	264	PEK	O01-C1-C2	-3.01	105.01	111.50
19	N	1524	PGV	C3-C2-C1	-3.01	102.68	113.62
23	C	525	CHD	C9-C11-C12	3.00	118.27	114.30
23	J	60	CHD	C19-C10-C9	-3.00	107.05	111.18
17	A	515	HEA	C16-C17-C18	3.00	121.74	111.88
25	C	264	PEK	C3-C2-C1	-2.99	102.75	113.62
17	N	515	HEA	C27-C19-C20	2.99	120.30	115.27
22	O	1230	PSC	C01-O03-C19	-2.98	106.08	117.12
25	P	1265	PEK	C11-C10-C9	2.98	126.69	112.02
26	G	269	CDL	C22-C21-C20	2.97	129.49	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	C10-O7-C3	2.96	125.28	117.96
23	G	86	CHD	C11-C12-C13	-2.95	108.21	111.24
25	P	1265	PEK	C24-C23-C22	2.95	123.80	113.19
25	C	265	PEK	P-O12-C04	2.95	136.10	121.59
17	A	516	HEA	C4B-C3B-C2B	-2.94	104.81	106.87
26	P	1270	CDL	OB6-CB5-C51	-2.94	105.17	111.50
25	P	1265	PEK	P-O11-C03	2.94	138.89	121.68
23	C	271	CHD	C11-C12-C13	2.93	114.25	111.24
24	M	526	DMU	C10-O1-C9	2.92	119.42	113.69
18	Y	1522	TGL	C13-C12-C11	2.92	129.26	114.42
18	A	523	TGL	OG1-CG1-CG2	2.92	116.92	108.43
19	C	268	PGV	C02-O01-C1	-2.91	110.62	117.79
23	P	1271	CHD	C15-C16-C17	2.91	110.91	105.13
24	P	1272	DMU	C10-O7-C3	2.91	125.17	117.96
25	C	264	PEK	C23-C22-C21	-2.91	103.04	113.62
18	A	523	TGL	OG2-CB1-CB2	-2.91	105.23	111.50
23	P	1525	CHD	O12-C12-C11	2.90	115.03	109.12
18	A	523	TGL	CG1-OG1-CA1	-2.90	106.39	117.12
17	A	515	HEA	C1B-C2B-C3B	-2.89	104.98	107.00
23	J	60	CHD	C19-C10-C5	-2.88	105.47	110.36
23	C	271	CHD	C9-C11-C12	2.86	118.08	114.30
17	N	515	HEA	C26-C15-C14	-2.86	116.35	123.68
25	G	1263	PEK	P-O12-C04	2.85	135.64	121.59
23	C	525	CHD	C17-C13-C14	2.85	102.96	100.09
18	A	521	TGL	CG3-CG2-CG1	2.84	118.50	111.79
17	A	516	HEA	C20-C19-C18	-2.82	115.41	121.12
25	T	1264	PEK	C3-C2-C1	-2.82	103.36	113.62
23	P	1271	CHD	C16-C15-C14	2.82	110.72	105.13
23	G	86	CHD	C9-C11-C12	2.82	118.02	114.30
25	C	264	PEK	C02-O01-C1	-2.80	110.89	117.79
24	M	526	DMU	C8-C7-C5	-2.80	105.94	110.82
23	C	525	CHD	C19-C10-C9	-2.80	107.33	111.18
23	B	1086	CHD	C14-C8-C7	-2.79	108.10	111.81
22	O	1230	PSC	P-O12-C04	2.79	135.33	121.59
25	C	265	PEK	C24-C23-C22	2.78	123.18	113.19
23	C	271	CHD	C15-C16-C17	2.78	110.64	105.13
23	P	1271	CHD	C11-C12-C13	2.75	114.07	111.24
24	M	526	DMU	O16-C6-C1	2.75	112.59	108.30
18	O	1521	TGL	CG3-CG2-CG1	2.74	118.28	111.79
23	W	1060	CHD	C14-C8-C7	2.74	115.44	111.81
18	A	523	TGL	OG2-CG2-CG3	2.73	118.27	108.40
18	A	523	TGL	OG3-CG3-CG2	-2.71	100.54	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	O	1521	TGL	C12-C11-C10	-2.71	100.67	114.42
19	A	524	PGV	C02-O01-C1	2.70	124.45	117.79
24	Z	1526	DMU	C10-O1-C9	2.69	118.97	113.69
17	A	515	HEA	C12-C13-C14	-2.69	105.14	112.23
19	P	1268	PGV	C02-O01-C1	-2.69	111.18	117.79
25	T	263	PEK	P-O12-C04	2.68	134.80	121.59
18	L	522	TGL	C13-C12-C11	2.67	128.00	114.42
18	O	1521	TGL	CA8-CA7-CA6	-2.67	100.85	114.42
23	C	271	CHD	C1-C2-C3	2.67	113.89	110.47
17	N	515	HEA	OMA-CMA-C3A	-2.66	119.12	124.91
17	N	515	HEA	C12-C13-C14	-2.66	105.22	112.23
17	A	515	HEA	C21-C20-C19	-2.65	104.26	112.98
17	N	515	HEA	C21-C20-C19	-2.65	104.27	112.98
23	G	86	CHD	C14-C8-C9	-2.65	106.08	109.71
23	C	525	CHD	C4-C3-C2	2.65	113.71	110.55
25	C	265	PEK	C2-C3-C4	2.65	117.95	113.23
24	C	272	DMU	O1-C10-C5	2.64	115.94	110.35
23	G	86	CHD	O12-C12-C11	2.63	114.47	109.12
25	G	1263	PEK	C03-C02-C01	2.61	117.96	111.79
25	P	1265	PEK	C2-C3-C4	2.59	117.84	113.23
26	G	269	CDL	C23-C22-C21	2.59	127.55	114.42
25	C	264	PEK	O03-C21-C22	-2.58	103.82	111.91
23	J	60	CHD	C14-C8-C9	2.57	113.25	109.71
26	P	1270	CDL	OA8-CA6-CA4	2.57	115.92	108.43
24	M	526	DMU	C6-C1-C2	2.57	115.34	110.00
25	C	264	PEK	C30-C29-C28	-2.56	101.44	114.42
26	P	1270	CDL	CB4-OB6-CB5	-2.55	111.51	117.79
18	A	521	TGL	C12-C11-C10	-2.54	101.52	114.42
25	T	1264	PEK	C30-C29-C28	-2.54	101.55	114.42
18	O	1521	TGL	OG3-CC1-CC2	-2.54	103.95	111.91
25	G	1263	PEK	C2-C3-C4	2.53	117.75	113.23
23	P	1525	CHD	C17-C13-C12	2.53	119.97	117.67
23	P	1271	CHD	C1-C2-C3	2.52	113.70	110.47
23	P	1525	CHD	C9-C11-C12	2.52	117.63	114.30
26	C	270	CDL	OB6-CB5-C51	-2.52	106.07	111.50
23	P	1525	CHD	C9-C10-C5	-2.52	105.04	108.58
25	P	1265	PEK	P-O12-C04	2.52	133.98	121.59
17	N	516	HEA	C27-C19-C20	2.52	119.51	115.27
23	P	1525	CHD	C4-C3-C2	2.50	113.54	110.55
23	B	1086	CHD	O12-C12-C11	2.50	114.22	109.12
26	T	1269	CDL	C23-C22-C21	2.50	127.10	114.42
23	W	1060	CHD	C5-C4-C3	2.49	116.41	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	1230	PSC	O03-C19-C20	-2.48	104.12	111.91
23	C	271	CHD	C2-C1-C10	2.48	117.03	112.78
25	T	1264	PEK	O03-C21-C22	-2.47	104.15	111.91
18	A	523	TGL	OG2-CG2-CG1	2.45	117.29	108.40
23	B	1086	CHD	C2-C1-C10	2.45	116.99	112.78
26	P	1270	CDL	OB6-CB5-OB7	2.44	129.59	123.70
18	A	521	TGL	OG3-CG3-CG2	2.43	115.50	108.43
23	W	1060	CHD	C14-C8-C9	2.42	113.04	109.71
23	J	60	CHD	C5-C4-C3	2.42	116.31	112.76
25	G	1263	PEK	C14-C13-C12	2.42	123.92	112.02
23	W	1060	CHD	O12-C12-C13	2.41	115.11	111.03
23	P	1271	CHD	C2-C1-C10	2.41	116.91	112.78
17	N	516	HEA	CMC-C2C-C1C	-2.41	124.77	128.46
17	N	515	HEA	C16-C17-C18	2.41	119.79	111.88
23	B	1086	CHD	C15-C16-C17	2.41	109.90	105.13
26	G	269	CDL	C83-C82-C81	2.40	126.63	114.42
23	B	1086	CHD	C11-C9-C10	2.40	116.20	113.73
26	C	270	CDL	C52-C51-CB5	-2.39	104.91	113.62
23	J	60	CHD	C14-C8-C7	2.39	114.98	111.81
18	A	521	TGL	OG2-CG2-CG3	2.39	117.06	108.40
25	C	264	PEK	O13-P-O14	2.38	124.01	112.24
26	G	269	CDL	C79-C78-C77	2.38	126.50	114.42
23	W	1060	CHD	O7-C7-C6	2.38	115.84	109.94
26	G	269	CDL	OA6-CA4-CA6	2.38	117.01	108.40
17	A	515	HEA	C20-C21-C22	2.37	119.67	111.88
23	G	86	CHD	C2-C1-C10	2.35	116.81	112.78
18	L	522	TGL	C20-CA9-CA8	2.35	126.34	114.42
23	C	525	CHD	C6-C5-C10	2.34	115.15	112.66
19	C	267	PGV	O01-C1-C2	-2.33	106.48	111.50
18	A	521	TGL	CA8-CA7-CA6	-2.33	102.62	114.42
19	C	268	PGV	O03-C01-C02	2.33	115.20	108.43
18	A	523	TGL	CC3-CC2-CC1	-2.32	105.19	113.62
23	J	60	CHD	C18-C13-C12	-2.32	106.71	109.07
18	L	522	TGL	CC7-CC6-CC5	2.31	126.16	114.42
26	T	1269	CDL	C19-C18-C17	2.31	126.16	114.42
26	C	270	CDL	OA8-CA6-CA4	2.31	115.15	108.43
24	Z	1526	DMU	C6-C1-C2	2.31	114.80	110.00
24	Z	1526	DMU	C8-C7-C5	-2.31	106.80	110.82
26	G	269	CDL	C19-C18-C17	2.30	126.12	114.42
23	J	60	CHD	C9-C11-C12	2.30	117.34	114.30
19	N	1524	PGV	C04-C05-C06	2.29	119.82	111.67
19	C	267	PGV	C03-C02-C01	2.29	117.20	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1264	PEK	O03-C01-C02	-2.28	101.78	108.43
26	C	270	CDL	C80-C79-C78	2.28	126.02	114.42
19	A	524	PGV	O01-C1-C2	-2.27	106.61	111.50
26	T	1269	CDL	C80-C79-C78	2.27	125.94	114.42
19	A	525	PGV	O01-C1-O02	2.27	129.18	123.70
18	A	521	TGL	CB7-CB6-CB5	-2.26	102.94	114.42
23	G	86	CHD	C11-C9-C10	2.26	116.06	113.73
18	Y	1522	TGL	C10-CB9-CB8	2.26	125.88	114.42
26	T	1269	CDL	C83-C82-C81	2.25	125.86	114.42
25	T	263	PEK	O03-C21-C22	2.25	118.97	111.91
19	P	1268	PGV	O03-C01-C02	2.24	114.96	108.43
17	A	515	HEA	C26-C15-C14	-2.24	117.93	123.68
26	G	269	CDL	C80-C79-C78	2.24	125.80	114.42
24	P	1272	DMU	O55-C2-C1	2.23	115.51	110.35
18	N	1523	TGL	OG2-CG2-CG1	2.23	116.48	108.40
26	T	1269	CDL	OB8-CB7-C71	-2.22	104.95	111.91
23	G	86	CHD	C15-C16-C17	2.21	109.51	105.13
18	A	521	TGL	OG3-CC1-CC2	-2.20	105.01	111.91
26	T	1269	CDL	C79-C78-C77	2.19	125.53	114.42
24	M	526	DMU	O7-C10-O1	2.19	116.78	110.67
18	A	521	TGL	C33-C19-C18	2.19	125.52	114.42
23	P	1271	CHD	C9-C11-C12	2.18	117.18	114.30
23	C	525	CHD	C16-C17-C13	-2.18	101.41	103.55
26	P	1270	CDL	C52-C51-CB5	-2.18	105.69	113.62
17	N	515	HEA	C20-C19-C18	2.18	125.53	121.12
23	G	86	CHD	C14-C8-C7	-2.17	108.92	111.81
22	B	230	PSC	O01-C1-C2	-2.17	106.81	111.50
25	T	1264	PEK	C24-C23-C22	-2.17	105.38	113.19
23	P	1271	CHD	O7-C7-C6	2.17	115.32	109.94
19	P	1267	PGV	C3-C2-C1	-2.17	105.73	113.62
18	N	1523	TGL	OG1-CG1-CG2	2.16	114.73	108.43
17	N	515	HEA	C20-C21-C22	2.15	118.95	111.88
23	G	86	CHD	C18-C13-C17	-2.15	107.85	111.21
23	B	1086	CHD	C4-C3-C2	2.14	113.11	110.55
19	P	1267	PGV	C9-C10-C11	-2.14	100.16	112.43
19	N	1524	PGV	C02-O01-C1	2.14	123.05	117.79
23	B	1086	CHD	O3-C3-C4	-2.13	105.61	109.85
25	T	263	PEK	C03-C02-C01	2.13	116.83	111.79
18	L	522	TGL	CC4-CC3-CC2	2.13	120.84	113.19
18	N	1523	TGL	CG3-CG2-CG1	-2.12	106.76	111.79
25	T	263	PEK	C14-C13-C12	2.12	122.46	112.02
22	O	1230	PSC	C07-N-C06	-2.11	103.56	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C18-C13-C17	-2.10	107.92	111.21
19	C	267	PGV	O12-P-O13	-2.10	100.86	109.07
24	C	272	DMU	O55-C2-C3	2.10	115.50	109.94
18	O	1521	TGL	C33-C19-C18	2.09	125.06	114.42
19	A	524	PGV	C04-C05-C06	2.08	119.07	111.67
24	C	272	DMU	C2-C3-C4	-2.08	106.16	110.93
23	C	525	CHD	C14-C13-C12	-2.08	105.47	107.40
18	O	1521	TGL	OG2-CG2-CG3	2.07	115.89	108.40
18	A	523	TGL	CA3-CA2-CA1	-2.07	106.10	113.62
26	T	1269	CDL	OB8-CB6-CB4	2.07	114.45	108.43
18	O	1521	TGL	CB9-CB8-CB7	-2.07	103.94	114.42
19	N	1524	PGV	O01-C1-C2	-2.06	107.06	111.50
25	C	264	PEK	O03-C21-O04	2.06	128.79	123.59
18	L	522	TGL	C14-C13-C12	-2.05	104.00	114.42
23	C	271	CHD	C6-C5-C4	-2.05	108.83	111.19
18	O	1521	TGL	CA3-CA2-CA1	-2.05	106.18	113.62
23	P	1271	CHD	O12-C12-C13	2.04	114.49	111.03
19	C	267	PGV	C9-C10-C11	-2.04	100.73	112.43
26	P	1270	CDL	C80-C79-C78	2.04	124.79	114.42
19	C	267	PGV	C3-C2-C1	-2.04	106.20	113.62
18	A	521	TGL	CA3-CA2-CA1	-2.04	106.20	113.62
23	J	60	CHD	O7-C7-C6	2.04	115.00	109.94
19	C	267	PGV	C02-O01-C1	-2.04	112.77	117.79
26	C	270	CDL	CB4-OB6-CB5	-2.04	112.77	117.79
26	T	1269	CDL	C20-C19-C18	2.04	124.77	114.42
18	A	523	TGL	CC4-CC3-CC2	-2.03	105.89	113.19
23	C	271	CHD	O7-C7-C6	2.02	114.96	109.94
18	L	522	TGL	CA9-CA8-CA7	2.02	124.69	114.42
18	Y	1522	TGL	C20-CA9-CA8	2.02	124.68	114.42
18	N	1523	TGL	CC3-CC2-CC1	-2.01	106.30	113.62
18	A	521	TGL	CA6-CA5-CA4	-2.00	104.27	114.42

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	P	1271	CHD	C12
23	P	1271	CHD	C8
23	P	1271	CHD	C3
23	P	1271	CHD	C9
23	P	1271	CHD	C14
23	J	60	CHD	C12
23	J	60	CHD	C8

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Mol	Chain	Res	Type	Atom
23	J	60	CHD	C9
23	J	60	CHD	C14
23	J	60	CHD	C17
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
24	C	272	DMU	C5
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C2
24	C	272	DMU	C10
24	P	1272	DMU	C5
24	P	1272	DMU	C6
24	P	1272	DMU	C9
24	P	1272	DMU	C4
24	P	1272	DMU	C2
24	P	1272	DMU	C10
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C9
24	Z	1526	DMU	C5
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
23	C	271	CHD	C12
23	C	271	CHD	C8
23	C	271	CHD	C3
23	C	271	CHD	C9
23	C	271	CHD	C14
23	W	1060	CHD	C12
23	W	1060	CHD	C8
23	W	1060	CHD	C9
23	W	1060	CHD	C14
23	W	1060	CHD	C17

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Mol	Chain	Res	Type	Atom
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C6
24	M	526	DMU	C9
24	M	526	DMU	C5

All (858) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	OB6-CB4-CB6-OB8
19	C	268	PGV	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O13
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	C04-C05-C06-O06
23	J	60	CHD	C16-C17-C20-C21
23	J	60	CHD	C16-C17-C20-C22
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
17	A	515	HEA	C21-C22-C23-C25
18	O	1521	TGL	CB2-CB1-OG2-CG2
24	Z	1526	DMU	O5-C6-O16-C18
18	A	521	TGL	CB2-CB1-OG2-CG2
25	C	265	PEK	C03-O11-P-O13
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14
25	P	1265	PEK	C03-O11-P-O13
25	P	1265	PEK	C04-O12-P-O13
19	P	1268	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O13
19	P	1268	PGV	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
17	N	515	HEA	C21-C22-C23-C25
19	A	524	PGV	C04-O12-P-O13
19	A	524	PGV	C04-O12-P-O14
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	C05-C04-O12-P
19	A	524	PGV	C04-C05-C06-O06
19	A	524	PGV	O05-C05-C06-O06
19	A	524	PGV	O02-C1-O01-C02
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
19	N	1524	PGV	C04-O12-P-O13
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
24	M	526	DMU	O5-C6-O16-C18
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
19	A	524	PGV	O04-C19-O03-C01
19	N	1524	PGV	O04-C19-O03-C01
19	A	524	PGV	C20-C19-O03-C01
19	N	1524	PGV	C20-C19-O03-C01
18	N	1523	TGL	OC1-CC1-OG3-CG3
18	A	523	TGL	OC1-CC1-OG3-CG3
26	P	1270	CDL	OA7-CA5-OA6-CA4
22	O	1230	PSC	O02-C1-O01-C02
22	B	230	PSC	O02-C1-O01-C02
18	A	521	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	OA7-CA5-OA6-CA4
18	N	1523	TGL	CC2-CC1-OG3-CG3
19	A	524	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C2-C1-O01-C02
17	N	516	HEA	C21-C22-C23-C25
17	A	516	HEA	C21-C22-C23-C25
17	A	515	HEA	C26-C15-C16-C17
17	N	515	HEA	C26-C15-C16-C17
17	A	515	HEA	C14-C15-C16-C17
17	N	515	HEA	C14-C15-C16-C17
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C80-C81-C82-C83
18	L	522	TGL	C21-C20-CA9-CA8
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C77-C78-C79-C80
18	Y	1522	TGL	C21-C20-CA9-CA8
18	A	521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C57-C58-C59-C60
26	G	269	CDL	C17-C18-C19-C20
26	G	269	CDL	C20-C21-C22-C23
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C77-C78-C79-C80
26	T	1269	CDL	C31-CA7-OA8-CA6
18	O	1521	TGL	CA2-CA1-OG1-CG1
18	A	521	TGL	CA2-CA1-OG1-CG1
18	A	523	TGL	CC2-CC1-OG3-CG3
26	G	269	CDL	C31-CA7-OA8-CA6
26	P	1270	CDL	C20-C21-C22-C23
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C57-C58-C59-C60
26	T	1269	CDL	C60-C61-C62-C63
26	T	1269	CDL	C80-C81-C82-C83
18	O	1521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C60-C61-C62-C63
26	C	270	CDL	C77-C78-C79-C80
26	C	270	CDL	C80-C81-C82-C83
26	G	269	CDL	C57-C58-C59-C60
26	G	269	CDL	C80-C81-C82-C83
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C60-C61-C62-C63
26	P	1270	CDL	C77-C78-C79-C80
26	C	270	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C60-C61-C62-C63
18	O	1521	TGL	OB1-CB1-OG2-CG2
18	L	522	TGL	OA1-CA1-OG1-CG1
18	O	1521	TGL	OA1-CA1-OG1-CG1
18	A	521	TGL	OA1-CA1-OG1-CG1
26	P	1270	CDL	C17-C18-C19-C20
26	T	1269	CDL	C37-C38-C39-C40
26	C	270	CDL	C17-C18-C19-C20
26	P	1270	CDL	C37-C38-C39-C40
26	T	1269	CDL	O1-C1-CA2-OA2
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	OA9-CA7-OA8-CA6
18	Y	1522	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	C11-CA5-OA6-CA4
22	O	1230	PSC	C2-C1-O01-C02
22	B	230	PSC	C2-C1-O01-C02
26	G	269	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	C37-C38-C39-C40
18	N	1523	TGL	C21-C20-CA9-CA8
18	L	522	TGL	C11-C10-CB9-CB8
18	Y	1522	TGL	C11-C10-CB9-CB8
18	O	1521	TGL	C11-C10-CB9-CB8
18	A	521	TGL	C11-C10-CB9-CB8
18	A	523	TGL	C21-C20-CA9-CA8
18	N	1523	TGL	C11-C10-CB9-CB8
18	L	522	TGL	C16-C15-CC9-CC8
18	Y	1522	TGL	C16-C15-CC9-CC8
18	O	1521	TGL	C21-C20-CA9-CA8
18	A	521	TGL	C21-C20-CA9-CA8
18	A	523	TGL	C11-C10-CB9-CB8
18	N	1523	TGL	C16-C15-CC9-CC8
18	A	523	TGL	C16-C15-CC9-CC8
23	J	60	CHD	C17-C20-C22-C23
23	W	1060	CHD	C17-C20-C22-C23
26	T	1269	CDL	OA7-CA5-OA6-CA4
17	A	515	HEA	C21-C22-C23-C24
17	N	516	HEA	C21-C22-C23-C24
17	N	515	HEA	C21-C22-C23-C24
23	J	60	CHD	C21-C20-C22-C23
23	W	1060	CHD	C21-C20-C22-C23
24	P	1272	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
18	L	522	TGL	CA2-CA1-OG1-CG1
18	Y	1522	TGL	CA2-CA1-OG1-CG1
23	J	60	CHD	C13-C17-C20-C21
23	W	1060	CHD	C13-C17-C20-C21
23	P	1271	CHD	C13-C17-C20-C22
23	J	60	CHD	C13-C17-C20-C22
23	C	271	CHD	C13-C17-C20-C22
23	W	1060	CHD	C13-C17-C20-C22
17	A	516	HEA	C21-C22-C23-C24
24	Z	1526	DMU	C3-C4-C57-O61
24	Z	1526	DMU	O6-C11-C9-C8
24	M	526	DMU	O6-C11-C9-C8
17	N	515	HEA	C17-C18-C19-C27
26	P	1270	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CB2-C1-CA2-OA2
19	A	524	PGV	O12-C04-C05-C06
26	C	270	CDL	CA2-C1-CB2-OB2
19	N	1524	PGV	O12-C04-C05-C06
26	G	269	CDL	CB2-C1-CA2-OA2
24	P	1272	DMU	C3-C4-C57-O61
18	N	1523	TGL	CA2-CA1-OG1-CG1
22	O	1230	PSC	C20-C19-O03-C01
22	B	230	PSC	C20-C19-O03-C01
18	A	523	TGL	CA2-CA1-OG1-CG1
19	A	524	PGV	C19-C20-C21-C22
25	G	1263	PEK	C28-C29-C30-C31
25	T	263	PEK	C28-C29-C30-C31
19	A	524	PGV	O12-C04-C05-O05
19	N	1524	PGV	O12-C04-C05-O05
19	N	1524	PGV	C19-C20-C21-C22
24	C	272	DMU	C1-C6-O16-C18
24	P	1272	DMU	C1-C6-O16-C18
25	T	263	PEK	O03-C01-C02-O01
25	G	1263	PEK	O03-C01-C02-O01
24	M	526	DMU	C3-C4-C57-O61
25	T	263	PEK	C1-C2-C3-C4
22	O	1230	PSC	O04-C19-O03-C01
22	B	230	PSC	O04-C19-O03-C01
26	T	1269	CDL	C73-C74-C75-C76
22	B	230	PSC	C20-C21-C22-C23
26	G	269	CDL	C73-C74-C75-C76
24	C	272	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
25	G	1263	PEK	C1-C2-C3-C4
22	O	1230	PSC	C20-C21-C22-C23
25	C	264	PEK	C22-C21-O03-C01
26	G	269	CDL	OA7-CA5-OA6-CA4
26	C	270	CDL	CB7-C71-C72-C73
18	N	1523	TGL	OA1-CA1-OG1-CG1
25	C	264	PEK	O04-C21-O03-C01
18	A	523	TGL	OA1-CA1-OG1-CG1
26	P	1270	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CB2-OB2
19	C	268	PGV	O12-C04-C05-O05
19	P	1268	PGV	O12-C04-C05-O05
26	C	270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	O1-C1-CB2-OB2
25	T	1264	PEK	O04-C21-O03-C01
26	P	1270	CDL	CB7-C71-C72-C73
26	C	270	CDL	CA5-C11-C12-C13
24	C	272	DMU	O6-C11-C9-C8
19	C	268	PGV	C2-C1-O01-C02
19	P	1268	PGV	C2-C1-O01-C02
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CB2-OB2-PB2-OB5
25	T	263	PEK	C03-O11-P-O12
26	T	1269	CDL	CB3-OB5-PB2-OB2
25	G	1263	PEK	C03-O11-P-O12
25	C	265	PEK	C04-O12-P-O11
25	P	1265	PEK	C04-O12-P-O11
19	A	524	PGV	C04-O12-P-O11
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CB2-OB2-PB2-OB5
19	N	1524	PGV	C04-O12-P-O11
26	G	269	CDL	CB3-OB5-PB2-OB2
22	O	1230	PSC	C1-C2-C3-C4
22	B	230	PSC	C1-C2-C3-C4
24	C	272	DMU	O6-C11-C9-O1
18	Y	1522	TGL	CC2-CC3-CC4-CC5
25	T	1264	PEK	C22-C21-O03-C01
26	G	269	CDL	C15-C16-C17-C18
26	P	1270	CDL	CA5-C11-C12-C13
26	T	1269	CDL	CA2-C1-CB2-OB2
19	C	268	PGV	O12-C04-C05-C06
19	P	1268	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	CA2-C1-CB2-OB2
18	L	522	TGL	CC2-CC3-CC4-CC5
22	O	1230	PSC	C22-C23-C24-C25
18	L	522	TGL	CC3-CC4-CC5-CC6
22	B	230	PSC	C22-C23-C24-C25
19	P	1267	PGV	C22-C23-C24-C25
26	T	1269	CDL	C15-C16-C17-C18
26	T	1269	CDL	C58-C59-C60-C61
19	C	268	PGV	C24-C25-C26-C27
22	B	230	PSC	C29-C30-C31-C32
19	P	1267	PGV	C7-C8-C9-C10
19	A	524	PGV	C4-C5-C6-C7
19	N	1524	PGV	C4-C5-C6-C7
26	G	269	CDL	C58-C59-C60-C61
26	P	1270	CDL	C51-C52-C53-C54
25	T	263	PEK	C29-C30-C31-C32
26	T	1269	CDL	C56-C57-C58-C59
19	C	268	PGV	C13-C14-C15-C16
25	G	1263	PEK	C29-C30-C31-C32
19	C	267	PGV	C7-C8-C9-C10
19	C	267	PGV	C22-C23-C24-C25
22	O	1230	PSC	C29-C30-C31-C32
25	C	265	PEK	C25-C26-C27-C28
25	P	1265	PEK	C25-C26-C27-C28
19	P	1268	PGV	C24-C25-C26-C27
26	C	270	CDL	C51-C52-C53-C54
19	C	268	PGV	O02-C1-O01-C02
19	P	1268	PGV	O02-C1-O01-C02
26	P	1270	CDL	C59-C60-C61-C62
26	C	270	CDL	C59-C60-C61-C62
26	T	1269	CDL	C72-C73-C74-C75
19	N	1266	PGV	C29-C30-C31-C32
19	P	1268	PGV	C13-C14-C15-C16
26	G	269	CDL	C56-C57-C58-C59
26	G	269	CDL	C72-C73-C74-C75
26	P	1270	CDL	C16-C17-C18-C19
25	G	1263	PEK	C27-C28-C29-C30
19	A	525	PGV	C29-C30-C31-C32
25	T	263	PEK	C27-C28-C29-C30
26	C	270	CDL	C16-C17-C18-C19
17	A	515	HEA	C17-C18-C19-C27
25	P	1265	PEK	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	M	526	DMU	C25-C28-C31-C34
26	G	269	CDL	CA5-C11-C12-C13
19	N	1266	PGV	C7-C8-C9-C10
19	A	525	PGV	C7-C8-C9-C10
26	G	269	CDL	C13-C14-C15-C16
19	C	268	PGV	C22-C23-C24-C25
25	C	264	PEK	C31-C32-C33-C34
25	C	265	PEK	C16-C17-C18-C19
19	P	1268	PGV	C27-C28-C29-C30
26	C	270	CDL	C73-C74-C75-C76
19	P	1268	PGV	C04-C05-C06-O06
18	Y	1522	TGL	CC3-CC4-CC5-CC6
24	P	1272	DMU	C25-C28-C31-C34
19	A	524	PGV	C22-C23-C24-C25
26	T	1269	CDL	CA5-C11-C12-C13
25	T	1264	PEK	C1-C2-C3-C4
26	P	1270	CDL	C73-C74-C75-C76
26	P	1270	CDL	C75-C76-C77-C78
19	N	1266	PGV	C5-C6-C7-C8
24	Z	1526	DMU	C25-C28-C31-C34
19	P	1268	PGV	C22-C23-C24-C25
19	A	524	PGV	C28-C29-C30-C31
26	C	270	CDL	C75-C76-C77-C78
19	N	1524	PGV	C22-C23-C24-C25
24	P	1272	DMU	O5-C6-O16-C18
26	T	1269	CDL	C13-C14-C15-C16
19	C	268	PGV	C27-C28-C29-C30
19	N	1266	PGV	C6-C7-C8-C9
19	N	1266	PGV	C23-C24-C25-C26
19	A	525	PGV	C23-C24-C25-C26
19	N	1524	PGV	C28-C29-C30-C31
26	P	1270	CDL	C32-C33-C34-C35
26	C	270	CDL	C32-C33-C34-C35
25	T	1264	PEK	C31-C32-C33-C34
18	L	522	TGL	CB4-CB5-CB6-CB7
19	A	525	PGV	C5-C6-C7-C8
22	O	1230	PSC	C2-C3-C4-C5
18	Y	1522	TGL	CB4-CB5-CB6-CB7
22	B	230	PSC	C2-C3-C4-C5
26	C	270	CDL	C36-C37-C38-C39
19	A	525	PGV	C6-C7-C8-C9
26	P	1270	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	C16-C17-C18-C19
19	C	268	PGV	C3-C4-C5-C6
25	P	1265	PEK	C29-C30-C31-C32
26	P	1270	CDL	C36-C37-C38-C39
19	P	1268	PGV	C3-C4-C5-C6
26	C	270	CDL	C71-C72-C73-C74
24	P	1272	DMU	O6-C11-C9-C8
26	P	1270	CDL	C71-C72-C73-C74
19	N	1524	PGV	C24-C25-C26-C27
25	T	1264	PEK	C22-C23-C24-C25
23	P	1271	CHD	C13-C17-C20-C21
19	C	268	PGV	O05-C05-C06-O06
19	P	1268	PGV	O05-C05-C06-O06
19	C	268	PGV	C28-C29-C30-C31
24	C	272	DMU	C25-C28-C31-C34
25	C	265	PEK	C29-C30-C31-C32
19	P	1268	PGV	C28-C29-C30-C31
19	A	524	PGV	C20-C21-C22-C23
25	T	1264	PEK	C16-C17-C18-C19
26	G	269	CDL	C43-C44-C45-C46
25	P	1265	PEK	C21-C22-C23-C24
19	A	524	PGV	C24-C25-C26-C27
19	C	268	PGV	C30-C31-C32-C33
26	C	270	CDL	C74-C75-C76-C77
25	T	1264	PEK	C23-C24-C25-C26
19	P	1268	PGV	C30-C31-C32-C33
26	C	270	CDL	C55-C56-C57-C58
25	T	1264	PEK	C25-C26-C27-C28
26	P	1270	CDL	C72-C73-C74-C75
26	P	1270	CDL	C74-C75-C76-C77
19	N	1524	PGV	C20-C21-C22-C23
17	N	515	HEA	C17-C18-C19-C20
25	C	264	PEK	C23-C24-C25-C26
25	C	264	PEK	C25-C26-C27-C28
26	C	270	CDL	C13-C14-C15-C16
26	G	269	CDL	C79-C80-C81-C82
26	T	1269	CDL	C43-C44-C45-C46
26	T	1269	CDL	C79-C80-C81-C82
25	C	265	PEK	C21-C22-C23-C24
26	P	1270	CDL	C13-C14-C15-C16
26	C	270	CDL	C72-C73-C74-C75
25	G	1263	PEK	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
23	C	271	CHD	C13-C17-C20-C21
19	P	1268	PGV	O04-C19-O03-C01
23	C	271	CHD	C16-C17-C20-C22
19	C	268	PGV	C11-C10-C9-C8
22	O	1230	PSC	C13-C14-C15-C16
22	B	230	PSC	C13-C14-C15-C16
19	P	1267	PGV	C11-C10-C9-C8
19	P	1268	PGV	C11-C10-C9-C8
19	P	1268	PGV	C20-C19-O03-C01
22	O	1230	PSC	C27-C28-C29-C30
26	C	270	CDL	C38-C39-C40-C41
26	P	1270	CDL	C18-C19-C20-C21
25	C	264	PEK	C22-C23-C24-C25
19	C	267	PGV	C13-C14-C15-C16
25	C	265	PEK	C31-C32-C33-C34
25	C	264	PEK	C1-C2-C3-C4
26	P	1270	CDL	C38-C39-C40-C41
25	T	263	PEK	C25-C26-C27-C28
19	C	268	PGV	C25-C26-C27-C28
19	P	1267	PGV	C13-C14-C15-C16
26	C	270	CDL	C18-C19-C20-C21
23	P	1271	CHD	C16-C17-C20-C21
25	T	263	PEK	C34-C35-C36-C37
24	C	272	DMU	O5-C6-O16-C18
22	B	230	PSC	C27-C28-C29-C30
26	C	270	CDL	C63-C64-C65-C66
26	P	1270	CDL	C51-CB5-OB6-CB4
26	P	1270	CDL	C63-C64-C65-C66
19	P	1267	PGV	C25-C26-C27-C28
26	G	269	CDL	C21-C22-C23-C24
18	L	522	TGL	OB1-CB1-OG2-CG2
19	P	1268	PGV	C1-C2-C3-C4
26	G	269	CDL	CB5-C51-C52-C53
26	P	1270	CDL	C34-C35-C36-C37
26	C	270	CDL	C42-C43-C44-C45
18	N	1523	TGL	OG2-CG2-CG3-OG3
18	A	523	TGL	OG2-CG2-CG3-OG3
19	C	267	PGV	C23-C24-C25-C26
26	C	270	CDL	C34-C35-C36-C37
26	T	1269	CDL	C21-C22-C23-C24
26	T	1269	CDL	C31-C32-C33-C34
25	T	263	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
19	P	1268	PGV	C25-C26-C27-C28
26	T	1269	CDL	C82-C83-C84-C85
25	G	1263	PEK	C34-C35-C36-C37
19	C	267	PGV	C25-C26-C27-C28
26	G	269	CDL	C31-C32-C33-C34
19	C	268	PGV	O04-C19-O03-C01
26	C	270	CDL	OB7-CB5-OB6-CB4
26	C	270	CDL	C51-CB5-OB6-CB4
25	G	1263	PEK	C26-C27-C28-C29
25	P	1265	PEK	C31-C32-C33-C34
19	N	1524	PGV	C5-C6-C7-C8
23	P	1271	CHD	C16-C17-C20-C22
26	G	269	CDL	C82-C83-C84-C85
25	T	263	PEK	C16-C17-C18-C19
19	C	268	PGV	C20-C19-O03-C01
26	T	1269	CDL	OA5-CA3-CA4-CA6
26	G	269	CDL	OA5-CA3-CA4-CA6
26	P	1270	CDL	C61-C62-C63-C64
22	O	1230	PSC	C23-C24-C25-C26
22	B	230	PSC	C23-C24-C25-C26
26	G	269	CDL	C14-C15-C16-C17
26	P	1270	CDL	OB7-CB5-OB6-CB4
18	Y	1522	TGL	OB1-CB1-OG2-CG2
19	P	1267	PGV	C23-C24-C25-C26
26	C	270	CDL	C61-C62-C63-C64
19	A	525	PGV	C25-C26-C27-C28
25	T	1264	PEK	C35-C36-C37-C38
19	C	268	PGV	C1-C2-C3-C4
23	C	271	CHD	C16-C17-C20-C21
26	P	1270	CDL	C42-C43-C44-C45
25	G	1263	PEK	C16-C17-C18-C19
26	P	1270	CDL	CB3-CB4-CB6-OB8
25	T	263	PEK	O03-C01-C02-C03
26	T	1269	CDL	CB3-CB4-CB6-OB8
25	G	1263	PEK	O03-C01-C02-C03
22	O	1230	PSC	O03-C01-C02-C03
22	B	230	PSC	O03-C01-C02-C03
26	C	270	CDL	CB3-CB4-CB6-OB8
25	T	1264	PEK	O03-C01-C02-C03
26	G	269	CDL	CB3-CB4-CB6-OB8
26	P	1270	CDL	C44-C45-C46-C47
22	B	230	PSC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	P	1267	PGV	C15-C16-C17-C18
19	C	268	PGV	C5-C6-C7-C8
19	C	267	PGV	C15-C16-C17-C18
22	O	1230	PSC	C3-C4-C5-C6
26	C	270	CDL	C44-C45-C46-C47
26	C	270	CDL	C64-C65-C66-C67
19	N	1266	PGV	C25-C26-C27-C28
26	C	270	CDL	C84-C85-C86-C87
19	C	267	PGV	C11-C10-C9-C8
26	T	1269	CDL	CB5-C51-C52-C53
25	T	1264	PEK	C32-C33-C34-C35
26	T	1269	CDL	C14-C15-C16-C17
22	O	1230	PSC	C14-C15-C16-C17
26	P	1270	CDL	C64-C65-C66-C67
19	C	267	PGV	C24-C25-C26-C27
26	T	1269	CDL	C35-C36-C37-C38
19	P	1267	PGV	C24-C25-C26-C27
19	P	1268	PGV	C5-C6-C7-C8
19	A	524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C03-C02-O01-C1
25	C	264	PEK	C24-C25-C26-C27
19	A	524	PGV	C5-C6-C7-C8
26	T	1269	CDL	C71-C72-C73-C74
25	C	264	PEK	C32-C33-C34-C35
24	Z	1526	DMU	C22-C25-C28-C31
25	T	1264	PEK	C27-C28-C29-C30
26	P	1270	CDL	C84-C85-C86-C87
26	T	1269	CDL	C33-C34-C35-C36
26	G	269	CDL	C33-C34-C35-C36
26	G	269	CDL	C53-C54-C55-C56
26	T	1269	CDL	C41-C42-C43-C44
26	T	1269	CDL	C53-C54-C55-C56
25	T	1264	PEK	C24-C25-C26-C27
25	G	1263	PEK	C15-C16-C17-C18
26	G	269	CDL	C71-C72-C73-C74
25	T	1264	PEK	O03-C01-C02-O01
19	C	268	PGV	C31-C32-C33-C34
26	G	269	CDL	C35-C36-C37-C38
26	G	269	CDL	C41-C42-C43-C44
18	Y	1522	TGL	CC5-CC6-CC7-CC8
18	L	522	TGL	CC5-CC6-CC7-CC8
18	Y	1522	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C30-C31-C32-C33
26	T	1269	CDL	C44-C45-C46-C47
18	A	521	TGL	CB6-CB7-CB8-CB9
19	P	1268	PGV	C31-C32-C33-C34
26	G	269	CDL	C44-C45-C46-C47
24	M	526	DMU	C22-C25-C28-C31
22	B	230	PSC	C3-C4-C5-C6
26	P	1270	CDL	OB5-CB3-CB4-CB6
26	C	270	CDL	OB5-CB3-CB4-CB6
24	C	272	DMU	C22-C25-C28-C31
25	C	264	PEK	C27-C28-C29-C30
19	P	1268	PGV	C14-C15-C16-C17
26	G	269	CDL	C19-C20-C21-C22
25	C	264	PEK	O03-C01-C02-C03
19	A	524	PGV	O03-C01-C02-C03
19	N	1524	PGV	O03-C01-C02-C03
26	P	1270	CDL	C43-C44-C45-C46
26	T	1269	CDL	C19-C20-C21-C22
25	G	1263	PEK	C30-C31-C32-C33
26	C	270	CDL	C39-C40-C41-C42
25	T	1264	PEK	C26-C27-C28-C29
22	O	1230	PSC	C11-C12-C13-C14
22	B	230	PSC	C11-C12-C13-C14
18	A	521	TGL	OC1-CC1-OG3-CG3
26	P	1270	CDL	C24-C25-C26-C27
25	C	264	PEK	C35-C36-C37-C38
19	P	1267	PGV	C20-C21-C22-C23
26	C	270	CDL	C24-C25-C26-C27
19	N	1266	PGV	C30-C31-C32-C33
19	A	525	PGV	C30-C31-C32-C33
25	T	263	PEK	C6-C7-C8-C9
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	G	1263	PEK	C6-C7-C8-C9
25	C	265	PEK	C11-C12-C13-C14
25	P	1265	PEK	C11-C12-C13-C14
25	T	1264	PEK	C5-C6-C7-C8
25	T	1264	PEK	C9-C10-C11-C12
26	G	269	CDL	CA7-C31-C32-C33
24	M	526	DMU	O5-C4-C57-O61
26	P	1270	CDL	C23-C24-C25-C26
19	C	268	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C23-C24-C25-C26
19	C	267	PGV	C20-C21-C22-C23
26	P	1270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OB5-CB3-CB4-OB6
19	C	268	PGV	O01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-OB6
25	T	263	PEK	C15-C16-C17-C18
26	P	1270	CDL	C39-C40-C41-C42
18	O	1521	TGL	OC1-CC1-OG3-CG3
26	P	1270	CDL	OB6-CB4-CB6-OB8
25	C	264	PEK	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
25	C	265	PEK	C35-C36-C37-C38
25	T	1264	PEK	C2-C1-O01-C02
17	N	515	HEA	C15-C16-C17-C18
19	P	1268	PGV	C23-C24-C25-C26
18	L	522	TGL	CC7-CC8-CC9-C15
22	O	1230	PSC	C31-C32-C33-C34
24	P	1272	DMU	C22-C25-C28-C31
25	T	263	PEK	C02-C03-O11-P
19	P	1267	PGV	C05-C04-O12-P
19	P	1268	PGV	C12-C13-C14-C15
19	N	1524	PGV	C12-C13-C14-C15
26	P	1270	CDL	C76-C77-C78-C79
26	T	1269	CDL	CA7-C31-C32-C33
25	C	264	PEK	C26-C27-C28-C29
19	C	268	PGV	C15-C16-C17-C18
18	O	1521	TGL	CB6-CB7-CB8-CB9
26	C	270	CDL	C43-C44-C45-C46
26	C	270	CDL	C76-C77-C78-C79
24	P	1272	DMU	O5-C4-C57-O61
25	T	1264	PEK	C17-C18-C19-C20
25	C	264	PEK	C17-C18-C19-C20
26	P	1270	CDL	C52-C53-C54-C55
26	P	1270	CDL	OA5-CA3-CA4-CA6
25	T	263	PEK	C01-C02-C03-O11
25	G	1263	PEK	C01-C02-C03-O11
22	B	230	PSC	C01-C02-C03-O11
19	N	1524	PGV	C01-C02-C03-O11
26	C	270	CDL	C52-C53-C54-C55
19	C	268	PGV	C12-C13-C14-C15
24	P	1272	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C34-C35-C36-C37
22	O	1230	PSC	C24-C25-C26-C27
19	P	1268	PGV	C15-C16-C17-C18
22	B	230	PSC	C24-C25-C26-C27
25	P	1265	PEK	C35-C36-C37-C38
18	L	522	TGL	CC2-CC1-OG3-CG3
25	T	263	PEK	C22-C21-O03-C01
25	G	1263	PEK	C22-C21-O03-C01
26	G	269	CDL	C54-C55-C56-C57
25	G	1263	PEK	C02-C03-O11-P
19	C	267	PGV	C05-C04-O12-P
26	G	269	CDL	CA3-CA4-CA6-OA8
26	T	1269	CDL	OA5-CA3-CA4-OA6
26	C	270	CDL	OA5-CA3-CA4-OA6
26	G	269	CDL	OA5-CA3-CA4-OA6
18	Y	1522	TGL	CC7-CC8-CC9-C15
26	C	270	CDL	C23-C24-C25-C26
24	Z	1526	DMU	O16-C18-C19-C22
25	T	263	PEK	O04-C21-O03-C01
25	G	1263	PEK	O04-C21-O03-C01
26	T	1269	CDL	OA6-CA4-CA6-OA8
19	A	524	PGV	O03-C01-C02-O01
26	G	269	CDL	OA6-CA4-CA6-OA8
18	A	521	TGL	CC2-CC1-OG3-CG3
25	T	263	PEK	C21-C22-C23-C24
26	T	1269	CDL	C54-C55-C56-C57
18	N	1523	TGL	CA9-C20-C21-C22
22	B	230	PSC	C31-C32-C33-C34
19	A	524	PGV	C12-C13-C14-C15
26	G	269	CDL	OB9-CB7-OB8-CB6
18	A	523	TGL	OB1-CB1-OG2-CG2
26	T	1269	CDL	OB9-CB7-OB8-CB6
26	G	269	CDL	C24-C25-C26-C27
24	Z	1526	DMU	O5-C4-C57-O61
25	G	1263	PEK	C21-C22-C23-C24
23	C	271	CHD	C17-C20-C22-C23
18	O	1521	TGL	CC2-CC1-OG3-CG3
25	C	265	PEK	C32-C33-C34-C35
19	P	1267	PGV	C31-C32-C33-C34
19	C	267	PGV	C31-C32-C33-C34
25	T	263	PEK	C03-O11-P-O13
25	G	1263	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C04-C05-N-C08
25	C	265	PEK	C03-O11-P-O14
25	P	1265	PEK	C03-O11-P-O14
22	O	1230	PSC	C01-C02-C03-O11
19	A	524	PGV	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6
25	C	265	PEK	C34-C35-C36-C37
18	A	521	TGL	C12-C13-C14-C29
25	T	263	PEK	C2-C3-C4-C5
26	T	1269	CDL	CB7-C71-C72-C73
25	G	1263	PEK	O01-C02-C03-O11
19	P	1268	PGV	C4-C5-C6-C7
19	A	524	PGV	C26-C27-C28-C29
26	C	270	CDL	C78-C79-C80-C81
24	M	526	DMU	C19-C18-O16-C6
18	A	523	TGL	CA9-C20-C21-C22
25	P	1265	PEK	C32-C33-C34-C35
26	T	1269	CDL	CA3-CA4-CA6-OA8
26	G	269	CDL	C78-C79-C80-C81
22	O	1230	PSC	O03-C01-C02-O01
22	B	230	PSC	O03-C01-C02-O01
19	N	1524	PGV	O03-C01-C02-O01
26	P	1270	CDL	C78-C79-C80-C81
26	T	1269	CDL	CB4-CB3-OB5-PB2
26	G	269	CDL	CB4-CB3-OB5-PB2
26	T	1269	CDL	C64-C65-C66-C67
19	C	268	PGV	C4-C5-C6-C7
25	G	1263	PEK	C2-C3-C4-C5
22	O	1230	PSC	C04-C05-N-C07
22	O	1230	PSC	C04-C05-N-C08
25	G	1263	PEK	C32-C33-C34-C35
26	T	1269	CDL	C24-C25-C26-C27
26	T	1269	CDL	C12-C13-C14-C15
25	G	1263	PEK	C31-C32-C33-C34
19	N	1524	PGV	C26-C27-C28-C29
26	T	1269	CDL	C36-C37-C38-C39
26	C	270	CDL	C11-C12-C13-C14
19	C	268	PGV	C01-C02-C03-O11
19	P	1268	PGV	C01-C02-C03-O11
25	T	263	PEK	C32-C33-C34-C35
26	G	269	CDL	C36-C37-C38-C39
25	T	263	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	C29-C30-C31-C32
25	P	1265	PEK	C3-C4-C5-C6
19	C	268	PGV	C02-C03-O11-P
19	P	1267	PGV	C02-C03-O11-P
25	T	263	PEK	O01-C02-C03-O11
19	P	1268	PGV	O01-C02-C03-O11
26	P	1270	CDL	C11-C12-C13-C14
24	M	526	DMU	C19-C22-C25-C28
22	B	230	PSC	C04-C05-N-C07
26	G	269	CDL	C12-C13-C14-C15
26	G	269	CDL	C64-C65-C66-C67
25	C	265	PEK	C3-C4-C5-C6
26	P	1270	CDL	CA3-OA5-PA1-OA2
25	C	265	PEK	C03-O11-P-O12
25	P	1265	PEK	C03-O11-P-O12
19	A	524	PGV	C03-O11-P-O12
26	C	270	CDL	CA3-OA5-PA1-OA2
19	N	1524	PGV	C03-O11-P-O12
17	A	515	HEA	C17-C18-C19-C20
18	A	521	TGL	CG2-CG3-OG3-CC1
19	N	1266	PGV	C9-C10-C11-C12
26	T	1269	CDL	C78-C79-C80-C81
18	N	1523	TGL	OB1-CB1-OG2-CG2
26	G	269	CDL	C38-C39-C40-C41
24	M	526	DMU	O16-C18-C19-C22
26	P	1270	CDL	C1-CA2-OA2-PA1
19	P	1268	PGV	C02-C03-O11-P
19	P	1268	PGV	C05-C04-O12-P
26	C	270	CDL	C1-CA2-OA2-PA1
25	T	263	PEK	C24-C25-C26-C27
19	A	525	PGV	C9-C10-C11-C12
26	C	270	CDL	C82-C83-C84-C85
26	G	269	CDL	CB7-C71-C72-C73
23	C	271	CHD	C21-C20-C22-C23
23	P	1271	CHD	C17-C20-C22-C23
18	O	1521	TGL	C12-C13-C14-C29
19	A	525	PGV	C26-C27-C28-C29
17	A	515	HEA	C15-C16-C17-C18
25	G	1263	PEK	C24-C25-C26-C27
19	N	1524	PGV	C11-C10-C9-C8
19	P	1267	PGV	C1-C2-C3-C4
25	C	265	PEK	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C30-C31-C32-C33
25	P	1265	PEK	C17-C18-C19-C20
22	O	1230	PSC	C21-C22-C23-C24
24	P	1272	DMU	C18-C19-C22-C25
26	P	1270	CDL	C41-C42-C43-C44
26	G	269	CDL	C22-C23-C24-C25
19	C	267	PGV	C02-C03-O11-P
26	T	1269	CDL	C59-C60-C61-C62
19	N	1266	PGV	C26-C27-C28-C29
26	T	1269	CDL	C22-C23-C24-C25
18	Y	1522	TGL	CB5-CB6-CB7-CB8
19	C	267	PGV	C29-C30-C31-C32
22	B	230	PSC	C21-C22-C23-C24
22	O	1230	PSC	C4-C5-C6-C7
26	C	270	CDL	CA3-CA4-CA6-OA8
26	G	269	CDL	C18-C19-C20-C21
22	O	1230	PSC	C03-C02-O01-C1
18	O	1521	TGL	CG1-CG2-OG2-CB1
22	B	230	PSC	C03-C02-O01-C1
18	A	521	TGL	CG1-CG2-OG2-CB1
26	T	1269	CDL	C38-C39-C40-C41
22	O	1230	PSC	C9-C10-C11-C12
22	B	230	PSC	C9-C10-C11-C12
19	C	268	PGV	C05-C04-O12-P
19	C	267	PGV	C14-C15-C16-C17
18	L	522	TGL	OG2-CB1-CB2-CB3
19	A	524	PGV	C11-C10-C9-C8
25	C	265	PEK	C30-C31-C32-C33
18	L	522	TGL	CB5-CB6-CB7-CB8
25	T	1264	PEK	C3-C4-C5-C6
24	C	272	DMU	C34-C37-C40-C43
19	A	524	PGV	C21-C22-C23-C24
26	P	1270	CDL	C15-C16-C17-C18
24	P	1272	DMU	C4-C3-O7-C10
18	Y	1522	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	CA3-CA4-CA6-OA8
23	P	1271	CHD	C21-C20-C22-C23
22	O	1230	PSC	C7-C8-C9-C10
19	A	524	PGV	C2-C3-C4-C5
22	O	1230	PSC	C04-C05-N-C06
22	B	230	PSC	C04-C05-N-C06
19	P	1267	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C3-C4-C5-C6
25	G	1263	PEK	C3-C4-C5-C6
26	T	1269	CDL	C18-C19-C20-C21
19	P	1268	PGV	C26-C27-C28-C29
18	Y	1522	TGL	OG3-CC1-CC2-CC3
24	Z	1526	DMU	C34-C37-C40-C43
22	O	1230	PSC	O03-C19-C20-C21
19	N	1524	PGV	O01-C1-C2-C3
22	B	230	PSC	C7-C8-C9-C10
19	P	1267	PGV	C21-C22-C23-C24
22	B	230	PSC	O03-C19-C20-C21
26	C	270	CDL	C52-C51-CB5-OB6
25	T	1264	PEK	O01-C1-C2-C3
19	N	1524	PGV	C25-C26-C27-C28
19	C	267	PGV	C1-C2-C3-C4
18	L	522	TGL	OG3-CC1-CC2-CC3
18	A	523	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C54-C55-C56-C57
26	P	1270	CDL	C52-C51-CB5-OB6
25	C	264	PEK	O01-C1-C2-C3
19	C	268	PGV	C26-C27-C28-C29
26	C	270	CDL	C15-C16-C17-C18
19	C	267	PGV	C21-C22-C23-C24
22	B	230	PSC	C4-C5-C6-C7
26	P	1270	CDL	C32-C31-CA7-OA8
19	A	524	PGV	O01-C1-C2-C3
26	C	270	CDL	C32-C31-CA7-OA8
26	P	1270	CDL	C83-C84-C85-C86
25	T	263	PEK	C14-C15-C16-C17
25	G	1263	PEK	C14-C15-C16-C17
19	C	267	PGV	C11-C12-C13-C14
19	P	1267	PGV	C11-C12-C13-C14
18	N	1523	TGL	OG2-CB1-CB2-CB3
19	N	1266	PGV	O03-C19-C20-C21
19	N	1524	PGV	C21-C22-C23-C24
26	C	270	CDL	C54-C55-C56-C57
18	A	523	TGL	CB2-CB3-CB4-CB5
22	O	1230	PSC	O01-C1-C2-C3
19	C	267	PGV	C9-C10-C11-C12
22	B	230	PSC	C12-C13-C14-C15
19	P	1267	PGV	C9-C10-C11-C12
18	O	1521	TGL	CG2-CG3-OG3-CC1

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Mol	Chain	Res	Type	Atoms
18	N	1523	TGL	C21-C22-C23-C24
18	N	1523	TGL	OG1-CG1-CG2-OG2
19	C	268	PGV	O03-C01-C02-O01
19	P	1268	PGV	O03-C01-C02-O01
18	A	523	TGL	OG1-CG1-CG2-OG2
26	T	1269	CDL	C62-C63-C64-C65
22	O	1230	PSC	C12-C13-C14-C15
19	N	1524	PGV	C9-C10-C11-C12
26	P	1270	CDL	C12-C11-CA5-OA6
18	A	523	TGL	OG3-CC1-CC2-CC3
26	G	269	CDL	C59-C60-C61-C62
19	N	1524	PGV	C2-C3-C4-C5
19	N	1266	PGV	C11-C12-C13-C14
22	B	230	PSC	O01-C1-C2-C3
22	B	230	PSC	O04-C19-C20-C21
18	O	1521	TGL	C13-C14-C29-C30
26	C	270	CDL	C12-C11-CA5-OA6
22	O	1230	PSC	O02-C1-C2-C3
19	A	524	PGV	C25-C26-C27-C28
18	N	1523	TGL	CB2-CB3-CB4-CB5
22	B	230	PSC	O02-C1-C2-C3
25	C	264	PEK	O02-C1-C2-C3
18	A	523	TGL	C21-C22-C23-C24
19	A	525	PGV	C11-C12-C13-C14
19	P	1267	PGV	C29-C30-C31-C32
26	P	1270	CDL	C82-C83-C84-C85
26	T	1269	CDL	C76-C77-C78-C79
26	P	1270	CDL	C32-C31-CA7-OA9
26	P	1270	CDL	C52-C51-CB5-OB7
19	A	524	PGV	O02-C1-C2-C3
19	N	1524	PGV	O02-C1-C2-C3
22	O	1230	PSC	O04-C19-C20-C21
18	A	523	TGL	OC1-CC1-CC2-CC3
25	T	1264	PEK	O02-C1-C2-C3
19	A	524	PGV	C9-C10-C11-C12
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	T	1269	CDL	CA2-OA2-PA1-OA3
19	C	267	PGV	C04-O12-P-O13
19	P	1267	PGV	C04-O12-P-O13
26	C	270	CDL	CA3-OA5-PA1-OA3
26	G	269	CDL	CA2-OA2-PA1-OA3
24	C	272	DMU	C4-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
18	N	1523	TGL	OC1-CC1-CC2-CC3
26	C	270	CDL	C32-C31-CA7-OA9
26	C	270	CDL	C52-C51-CB5-OB7
18	A	521	TGL	CB7-CB8-CB9-C10
18	N	1523	TGL	OG3-CC1-CC2-CC3
24	Z	1526	DMU	C19-C22-C25-C28
18	O	1521	TGL	C10-C11-C12-C13
19	A	525	PGV	O03-C19-C20-C21
18	Y	1522	TGL	CC6-CC7-CC8-CC9
19	P	1268	PGV	C7-C8-C9-C10
18	N	1523	TGL	CG3-CG2-OG2-CB1
18	A	523	TGL	CG3-CG2-OG2-CB1
18	Y	1522	TGL	C12-C13-C14-C29
26	T	1269	CDL	C55-C56-C57-C58
18	O	1521	TGL	OG1-CA1-CA2-CA3
25	C	265	PEK	C26-C27-C28-C29
26	G	269	CDL	C55-C56-C57-C58
25	P	1265	PEK	O03-C21-C22-C23
26	P	1270	CDL	CB2-C1-CA2-OA2
22	O	1230	PSC	O01-C02-C03-O11
22	B	230	PSC	O01-C02-C03-O11
19	N	1266	PGV	C31-C32-C33-C34
24	Z	1526	DMU	C19-C18-O16-C6
24	C	272	DMU	O5-C4-C57-O61
26	G	269	CDL	C62-C63-C64-C65
25	C	265	PEK	O03-C21-C22-C23
26	G	269	CDL	C71-CB7-OB8-CB6

There are no ring outliers.

41 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	1523	TGL	8	0
23	C	525	CHD	1	0
23	P	1271	CHD	5	0
26	P	1270	CDL	17	0
18	L	522	TGL	20	0
25	T	263	PEK	11	0
26	T	1269	CDL	32	0
25	P	1265	PEK	10	0
19	C	268	PGV	1	0
22	B	230	PSC	21	0

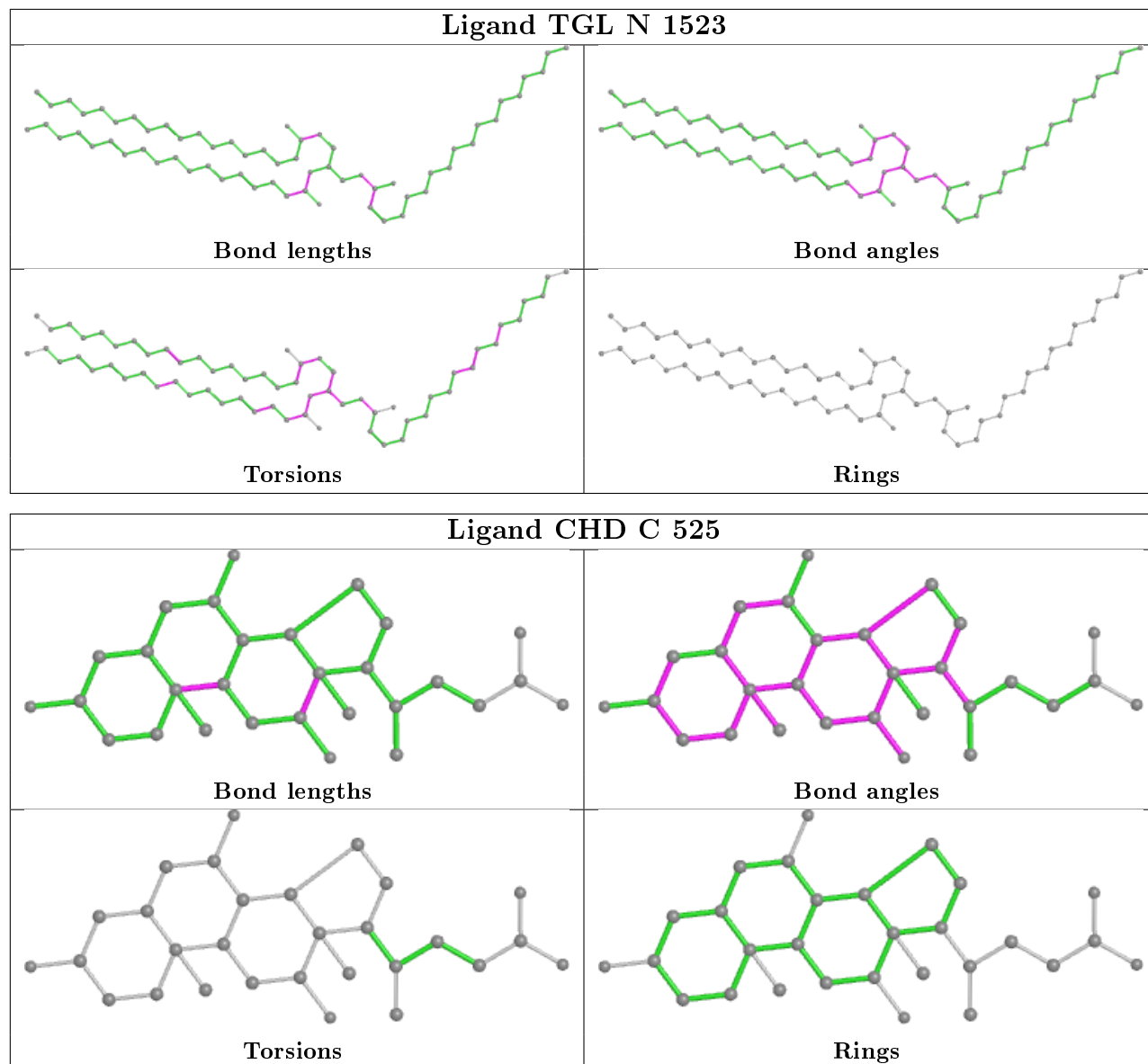
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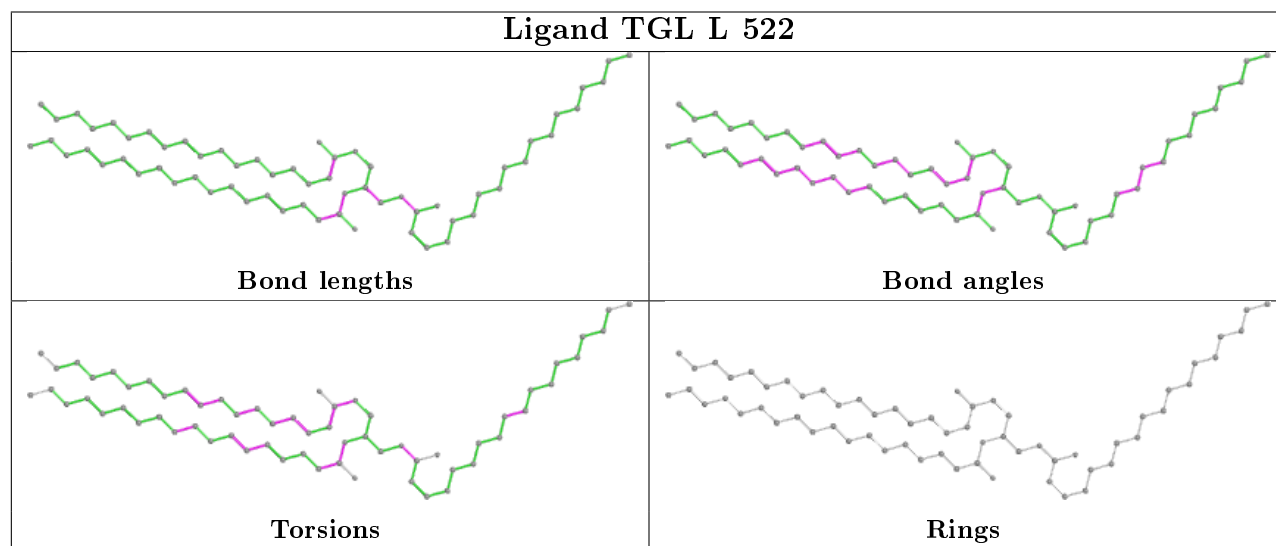
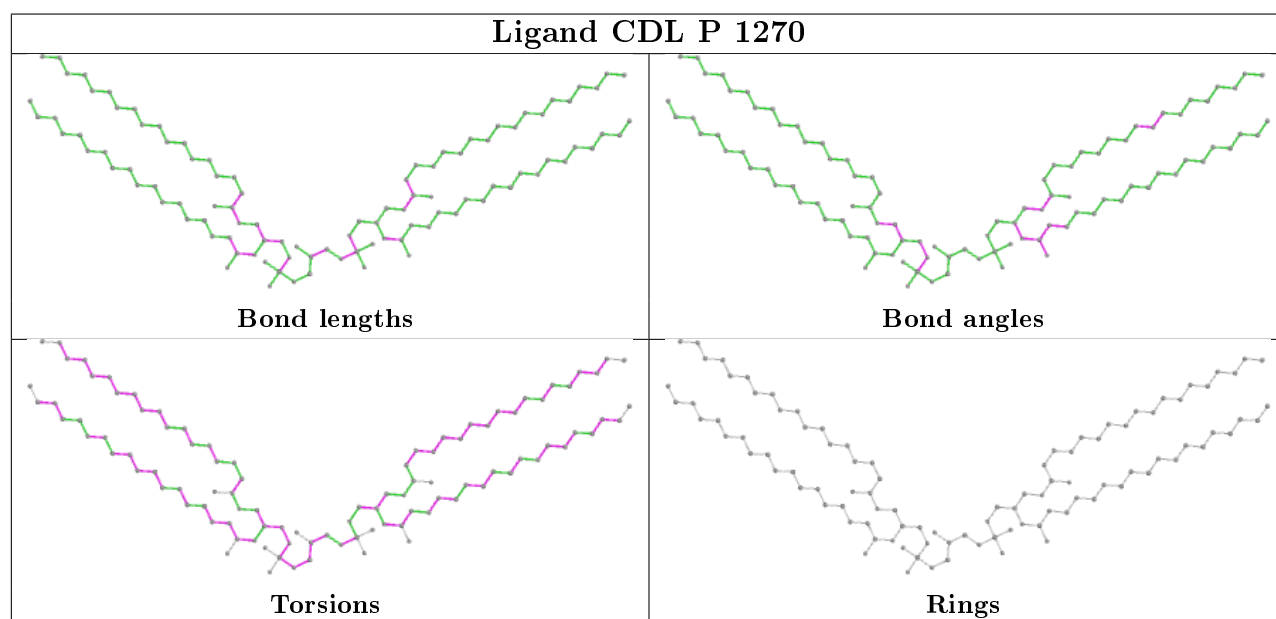
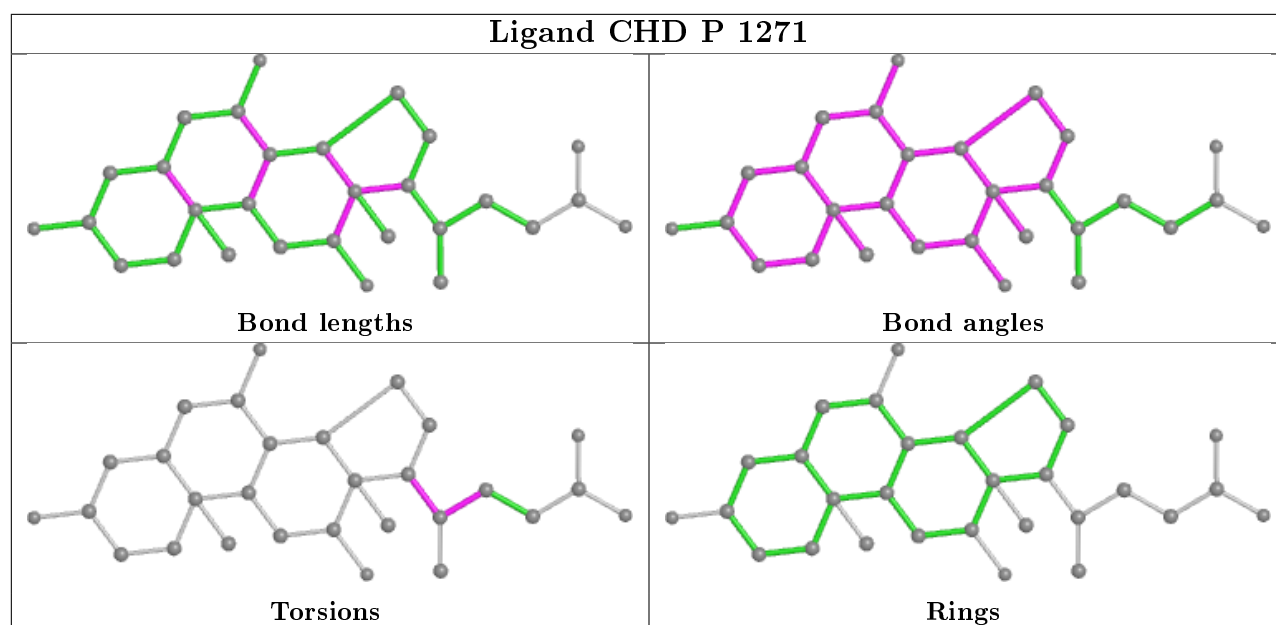
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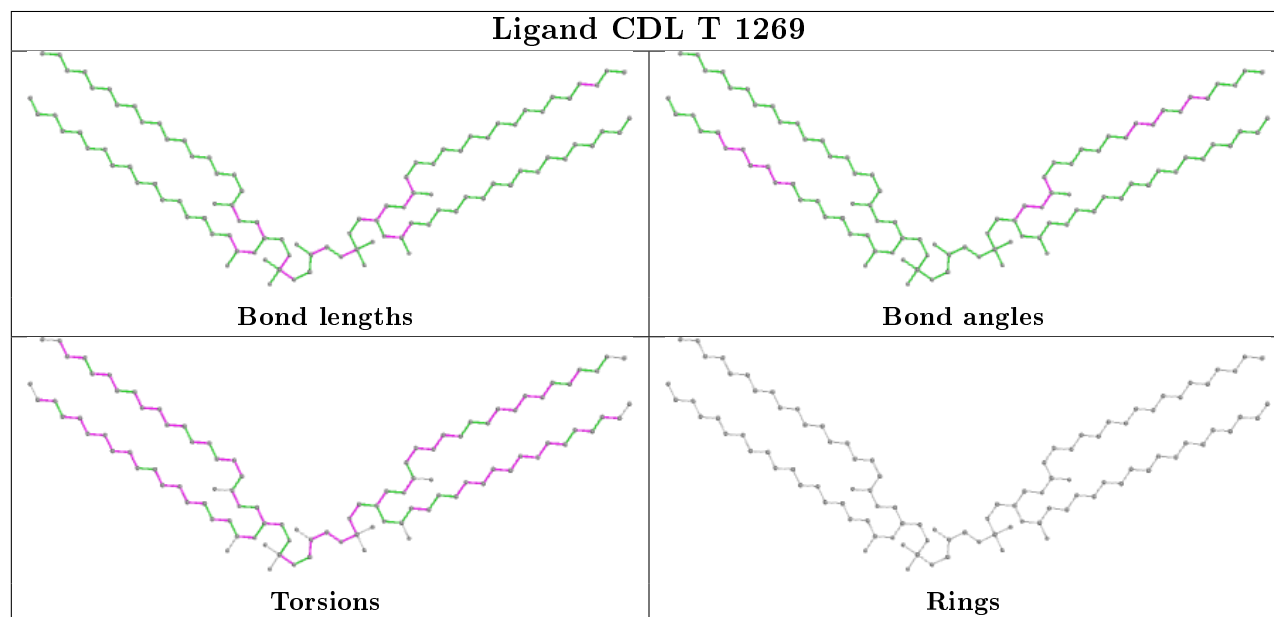
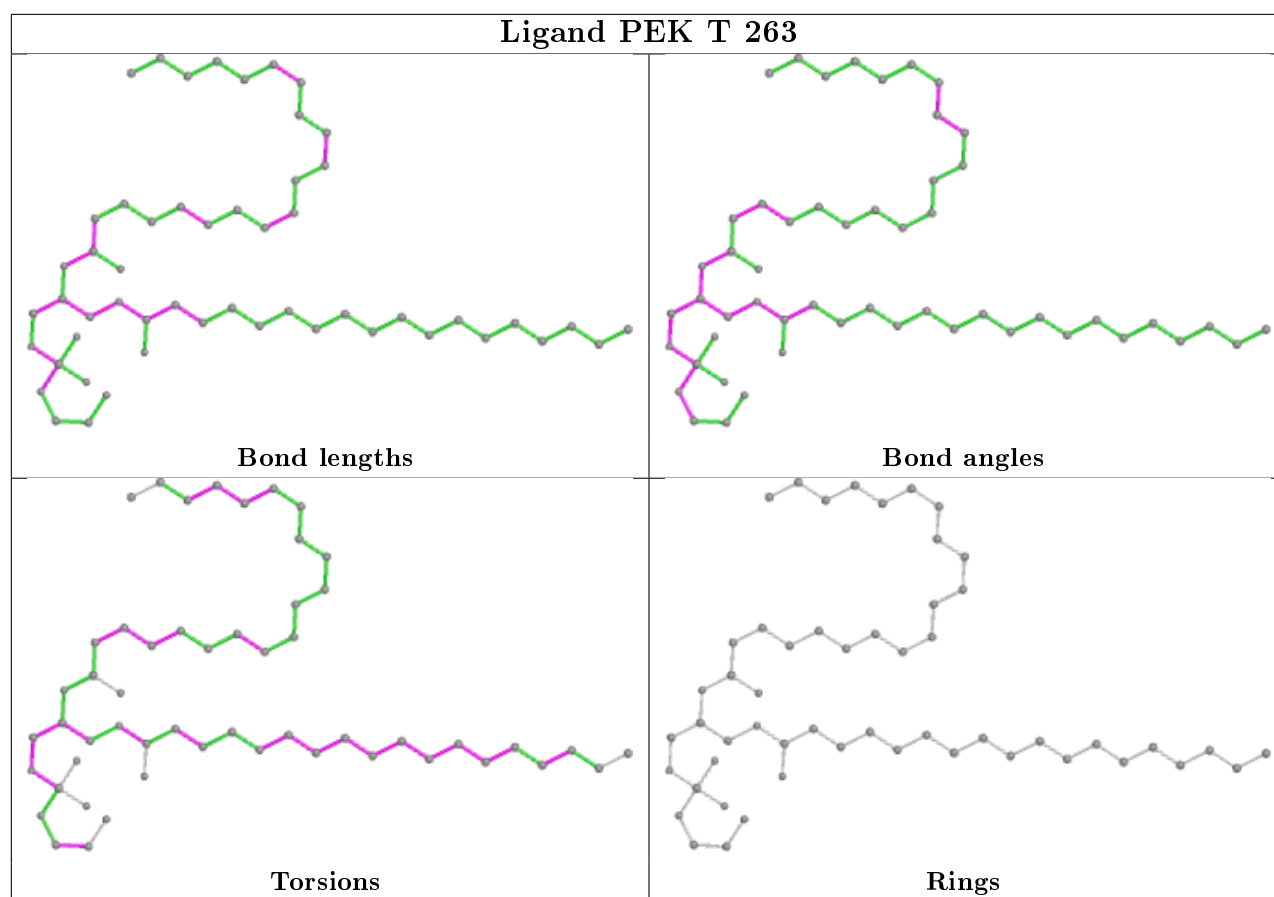
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	60	CHD	4	0
19	P	1267	PGV	9	0
25	C	264	PEK	9	0
25	G	1263	PEK	10	0
19	C	267	PGV	6	0
19	N	1266	PGV	2	0
22	O	1230	PSC	20	0
17	A	515	HEA	12	0
23	G	86	CHD	1	0
18	Y	1522	TGL	16	0
17	N	516	HEA	9	0
23	B	1086	CHD	5	0
18	O	1521	TGL	8	0
24	P	1272	DMU	4	0
23	W	1060	CHD	3	0
17	A	516	HEA	3	0
23	C	271	CHD	4	0
18	A	521	TGL	8	0
25	C	265	PEK	11	0
24	C	272	DMU	3	0
19	P	1268	PGV	2	0
17	N	515	HEA	9	0
25	T	1264	PEK	12	0
18	A	523	TGL	3	0
19	A	524	PGV	5	0
23	P	1525	CHD	1	0
26	C	270	CDL	17	0
19	A	525	PGV	4	0
19	N	1524	PGV	7	0
24	M	526	DMU	1	0
26	G	269	CDL	23	0

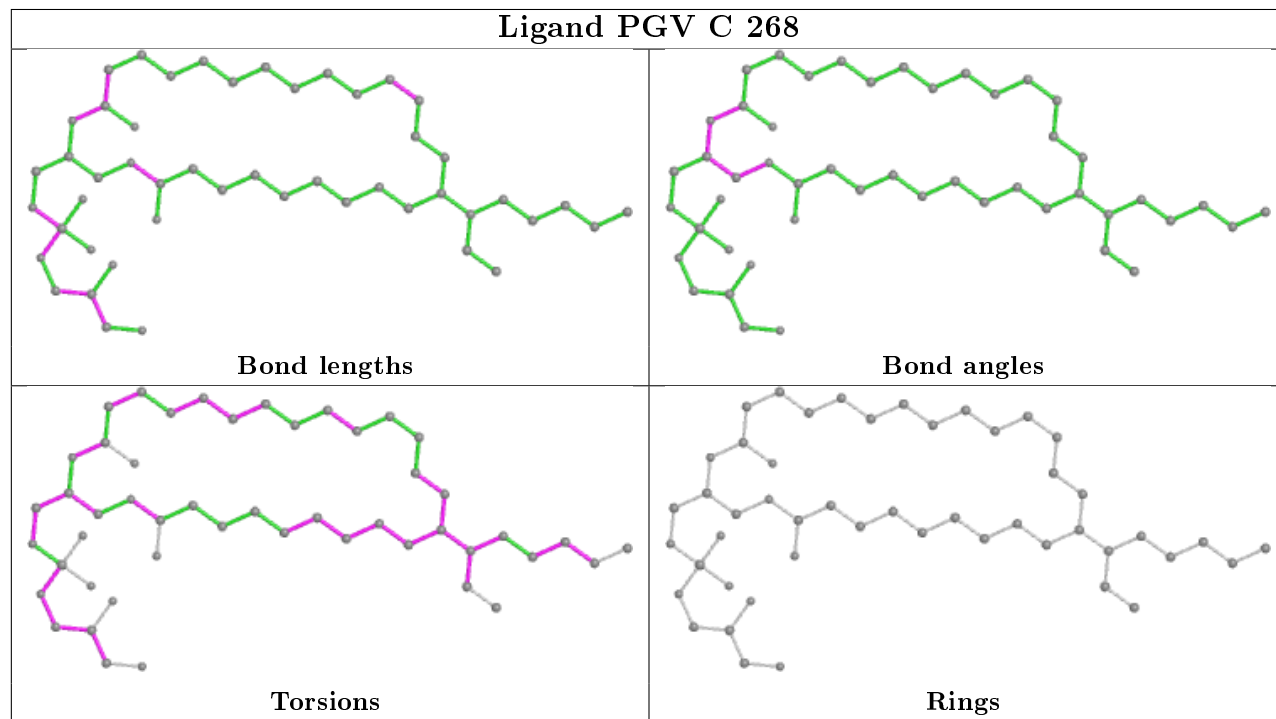
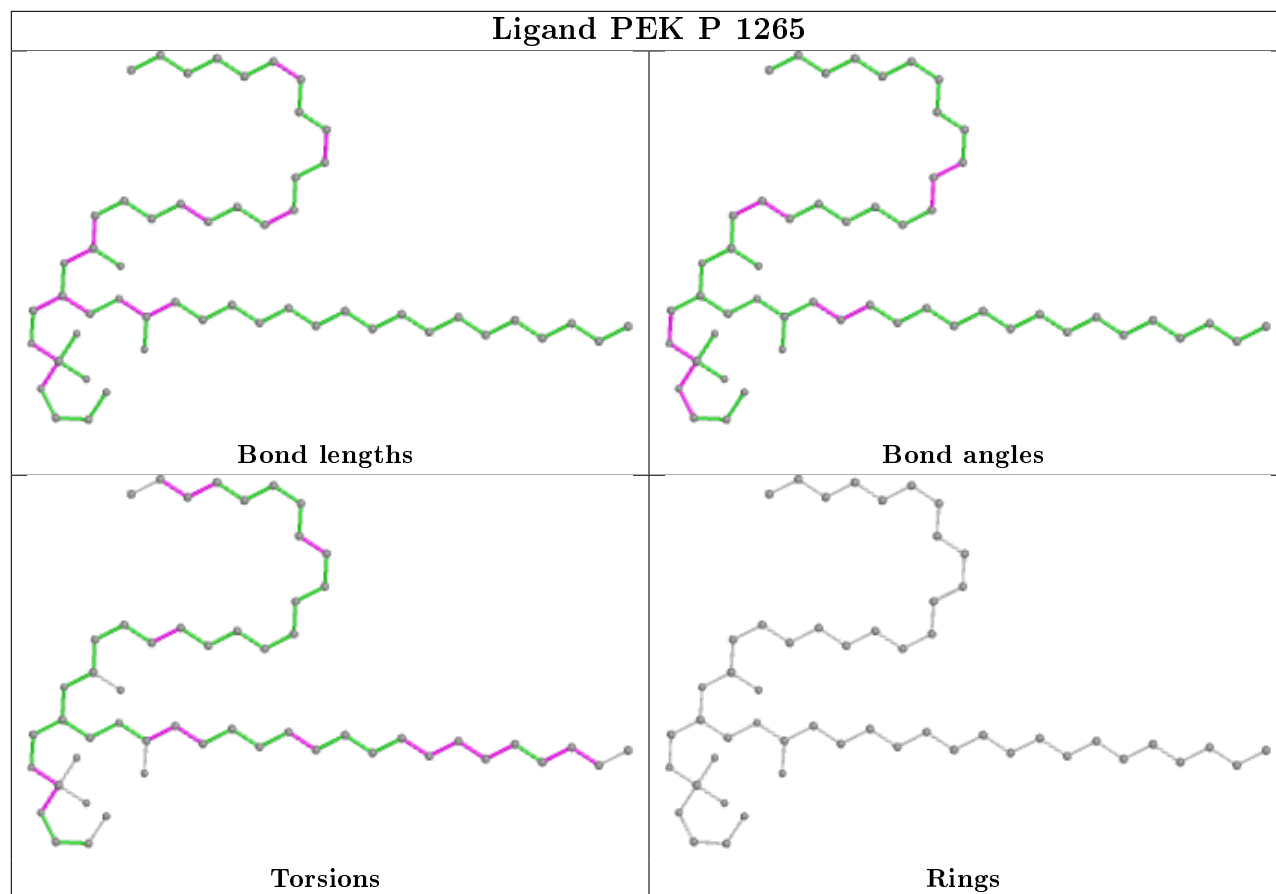
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

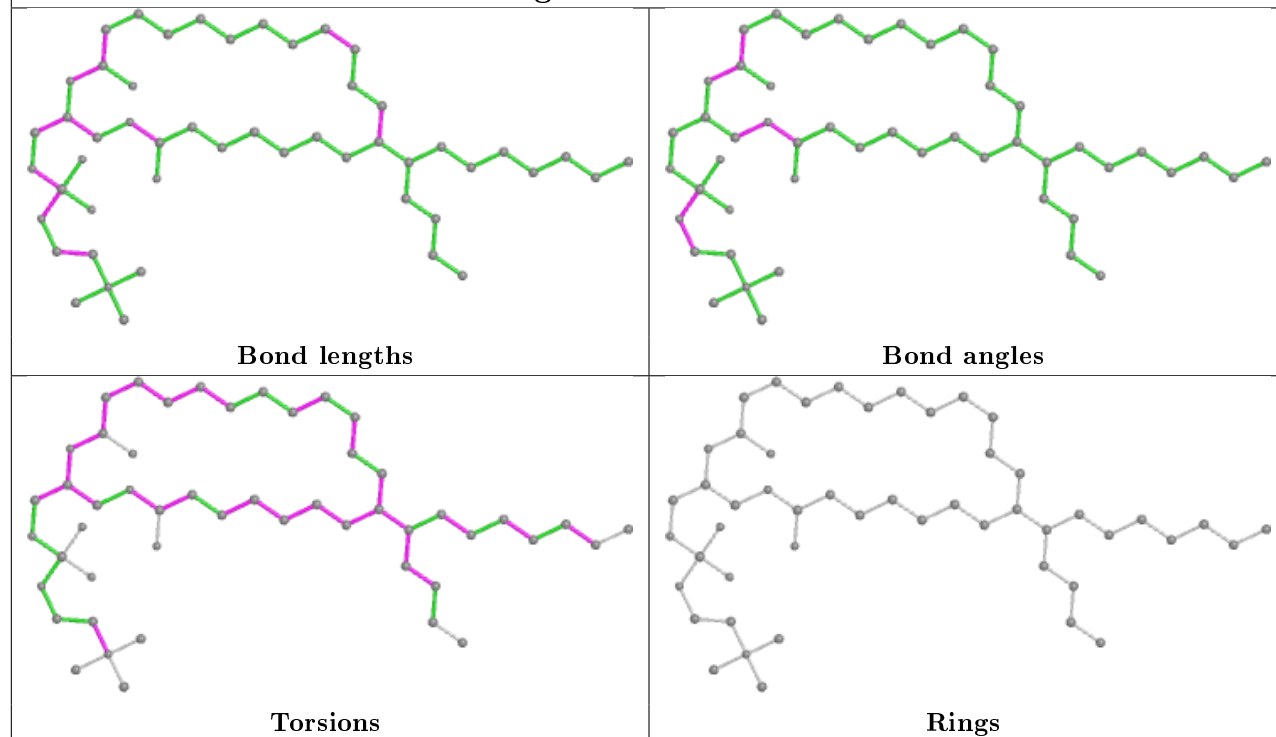




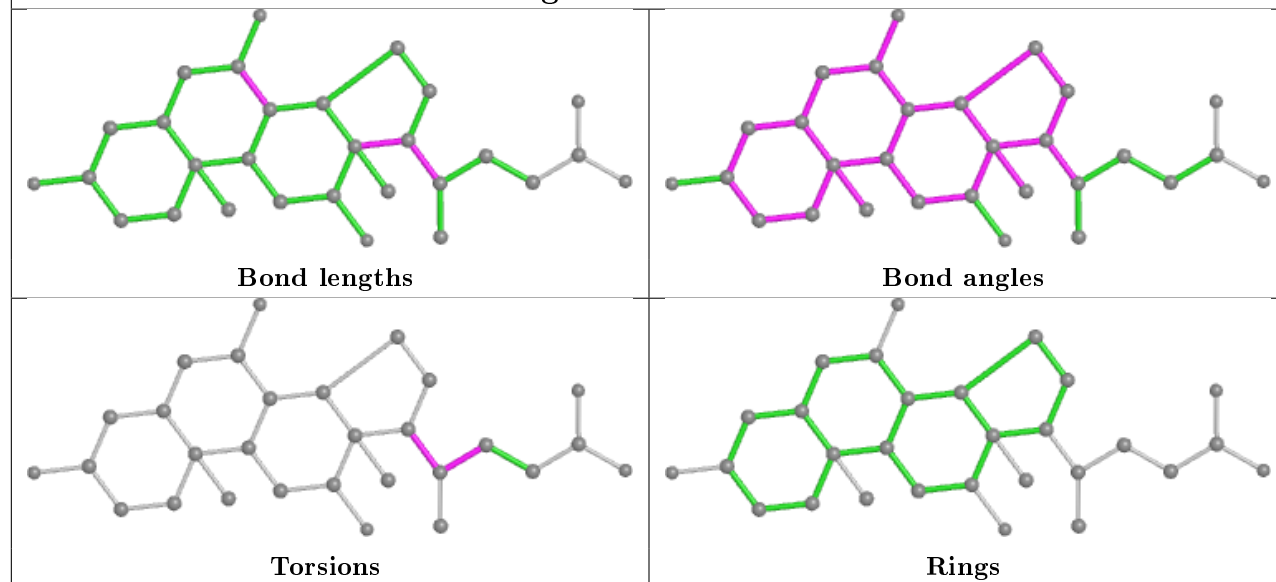




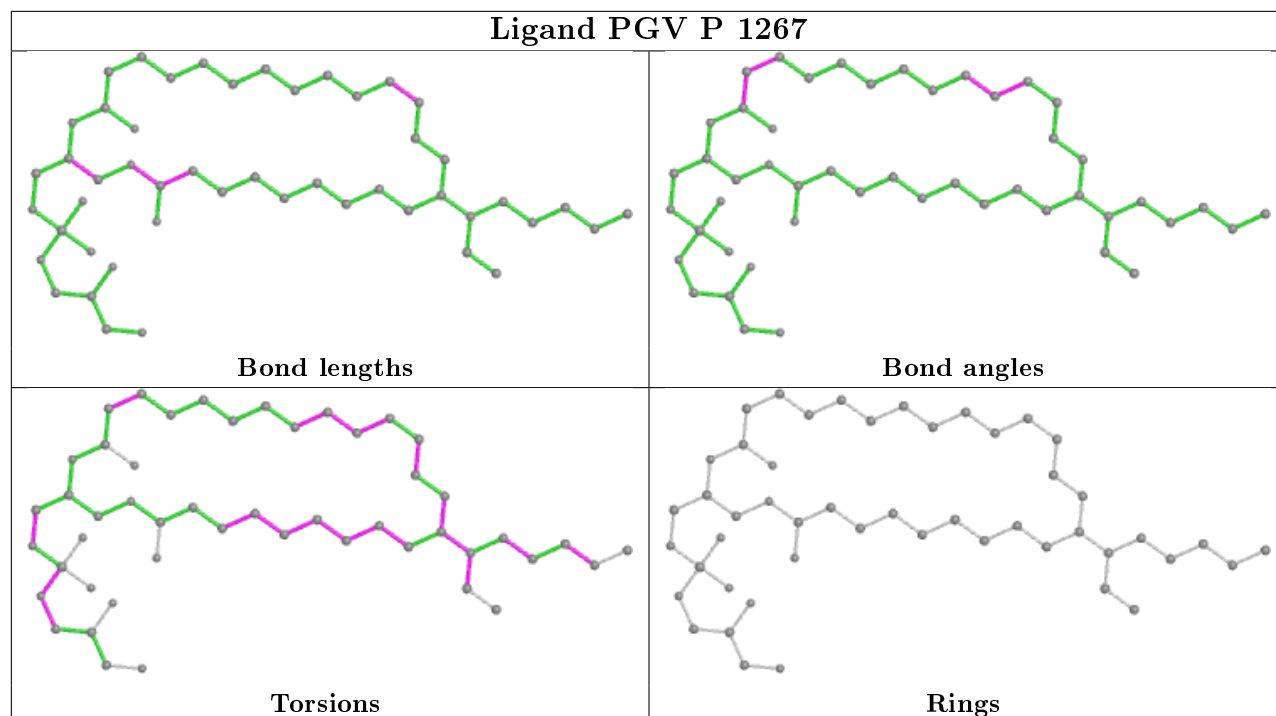
Ligand PSC B 230



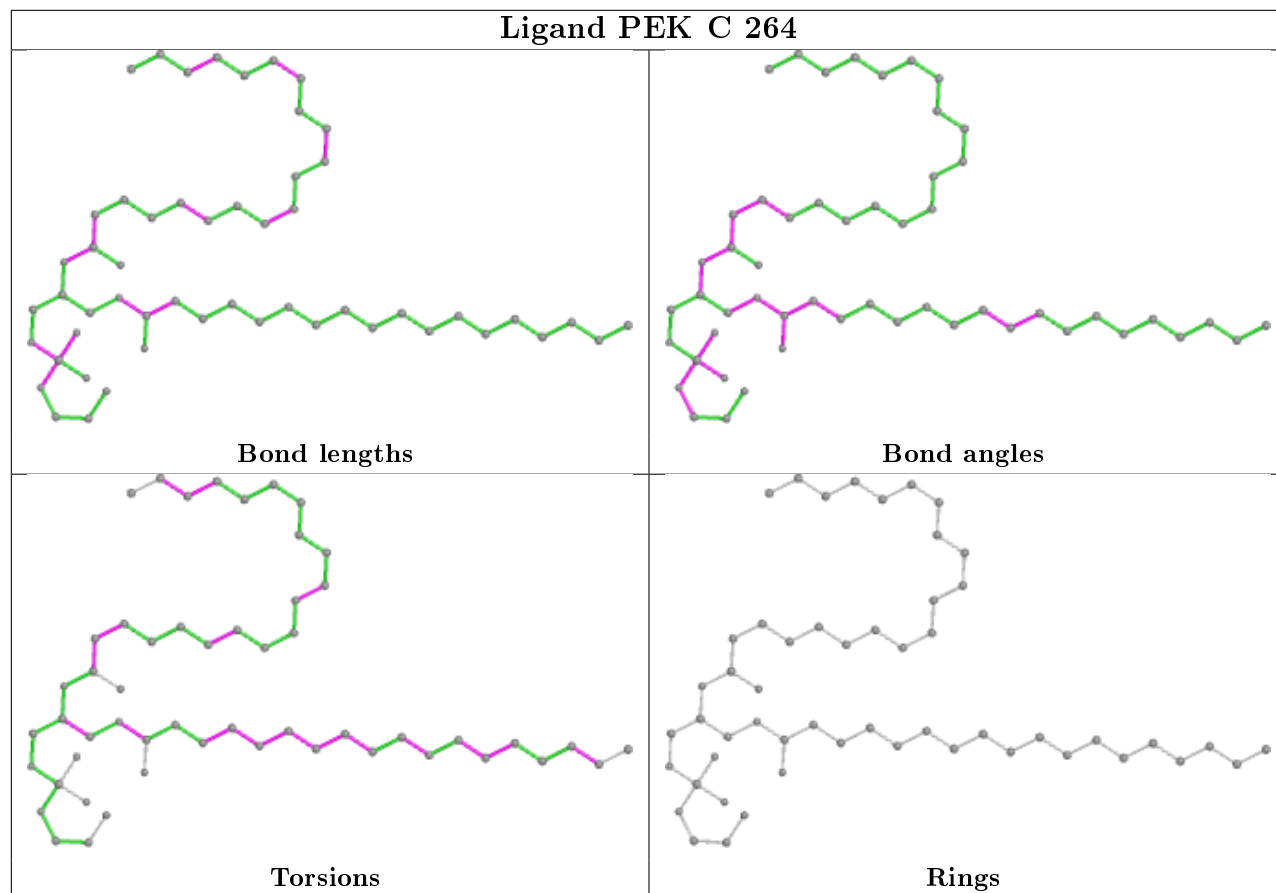
Ligand CHD J 60

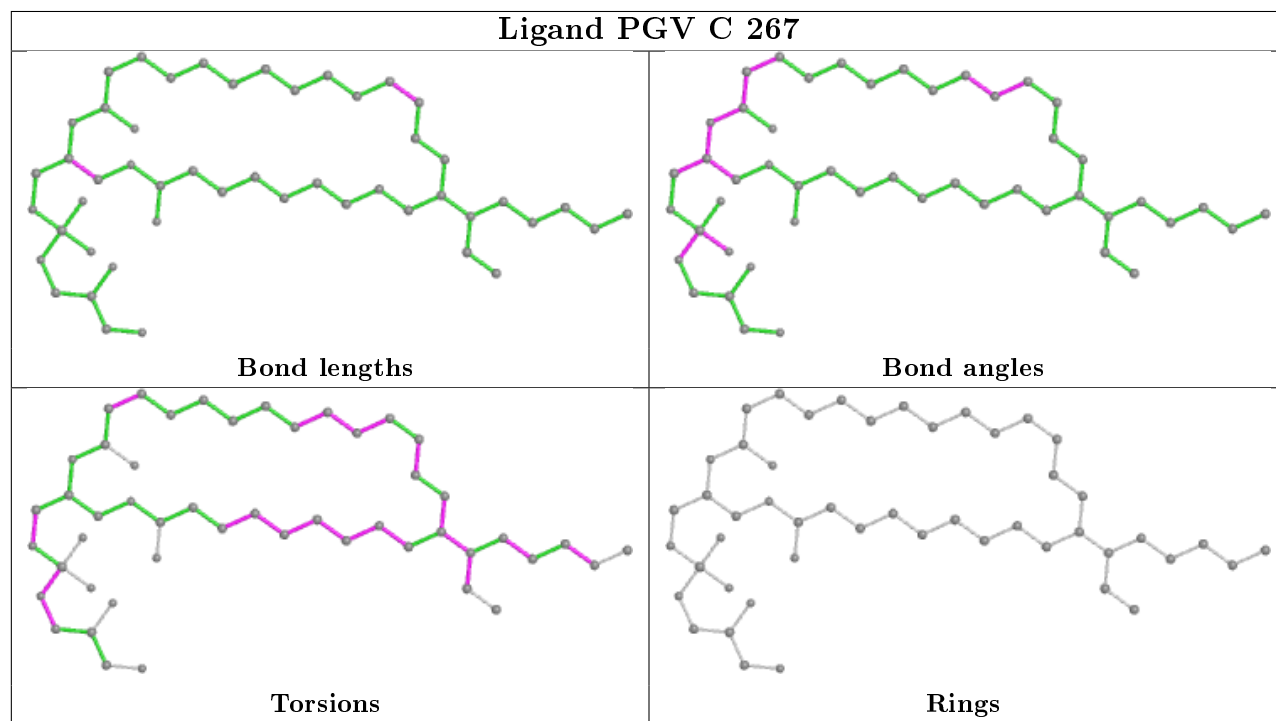
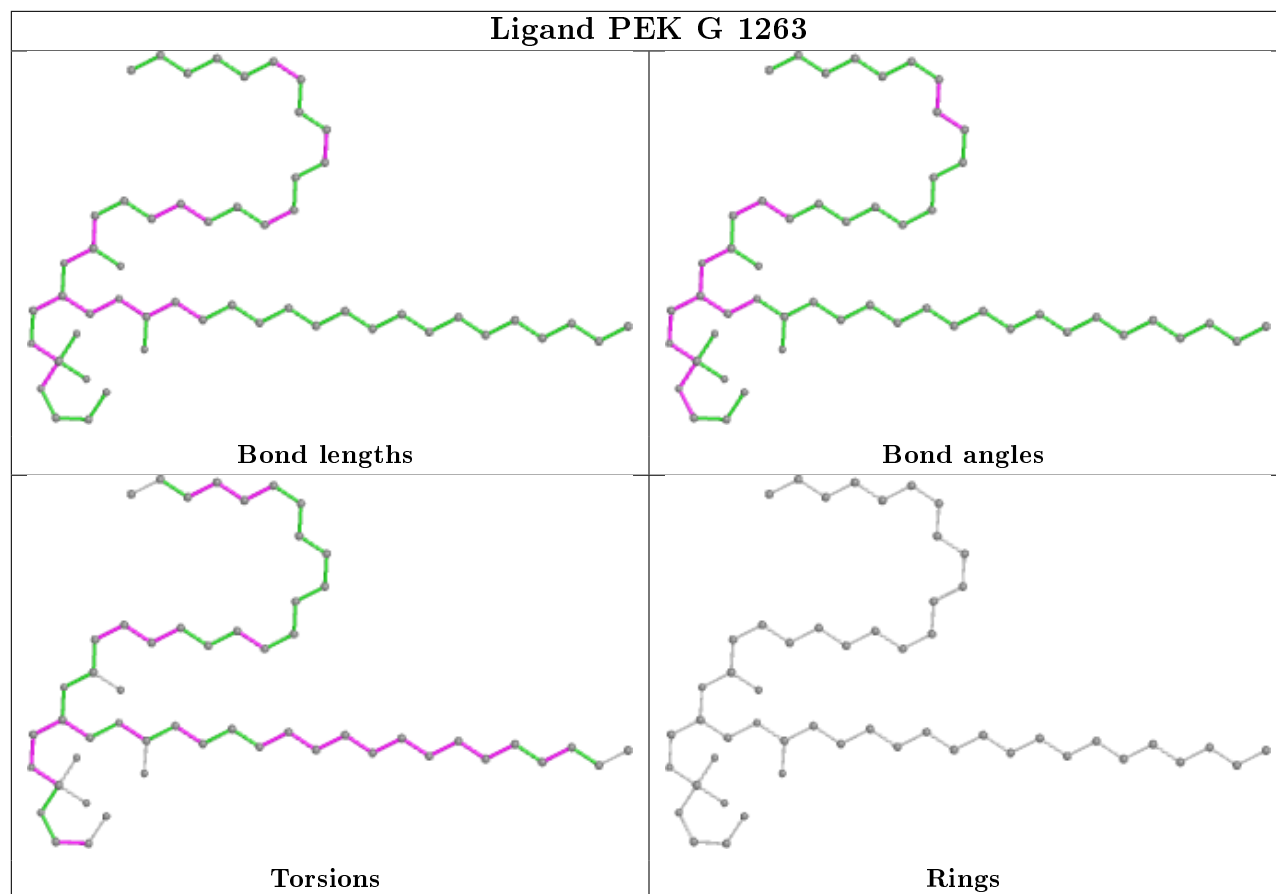


Ligand PGV P 1267

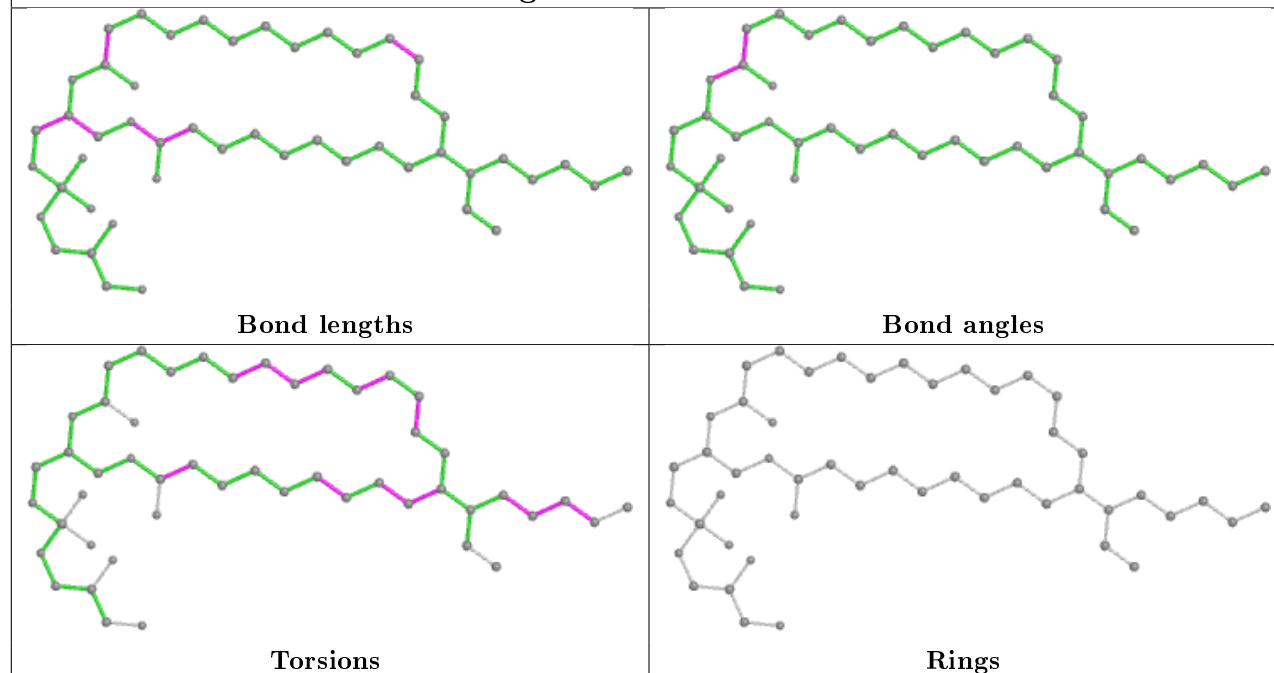


Ligand PEK C 264

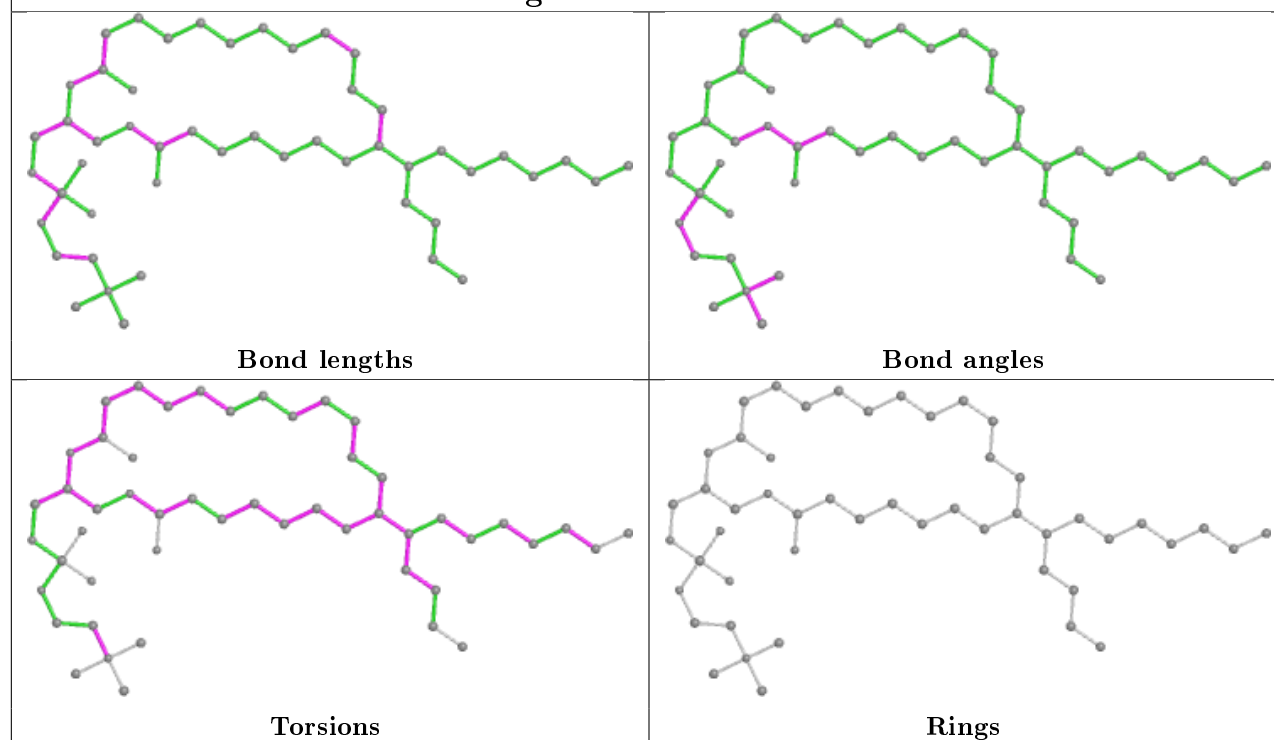


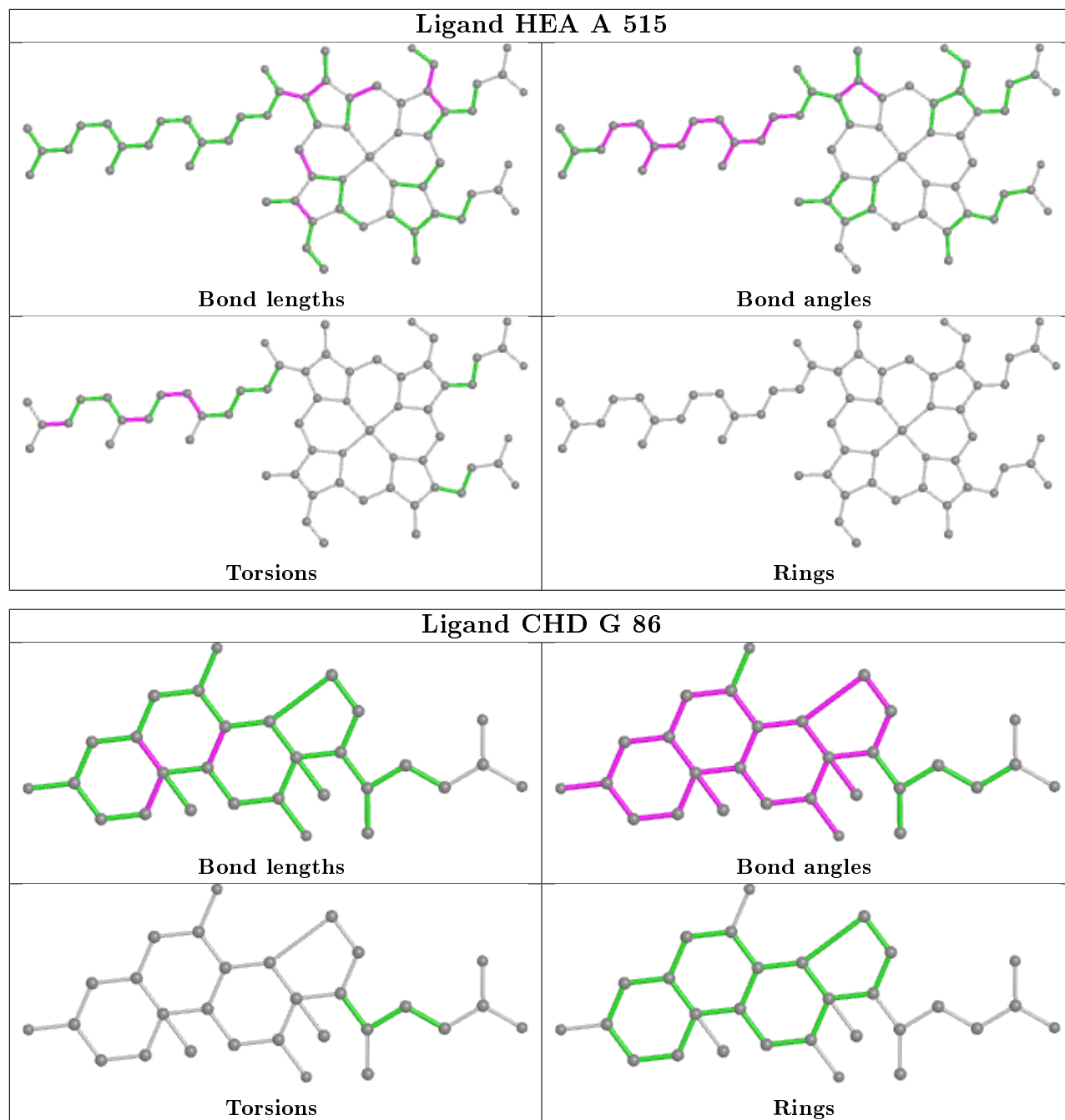


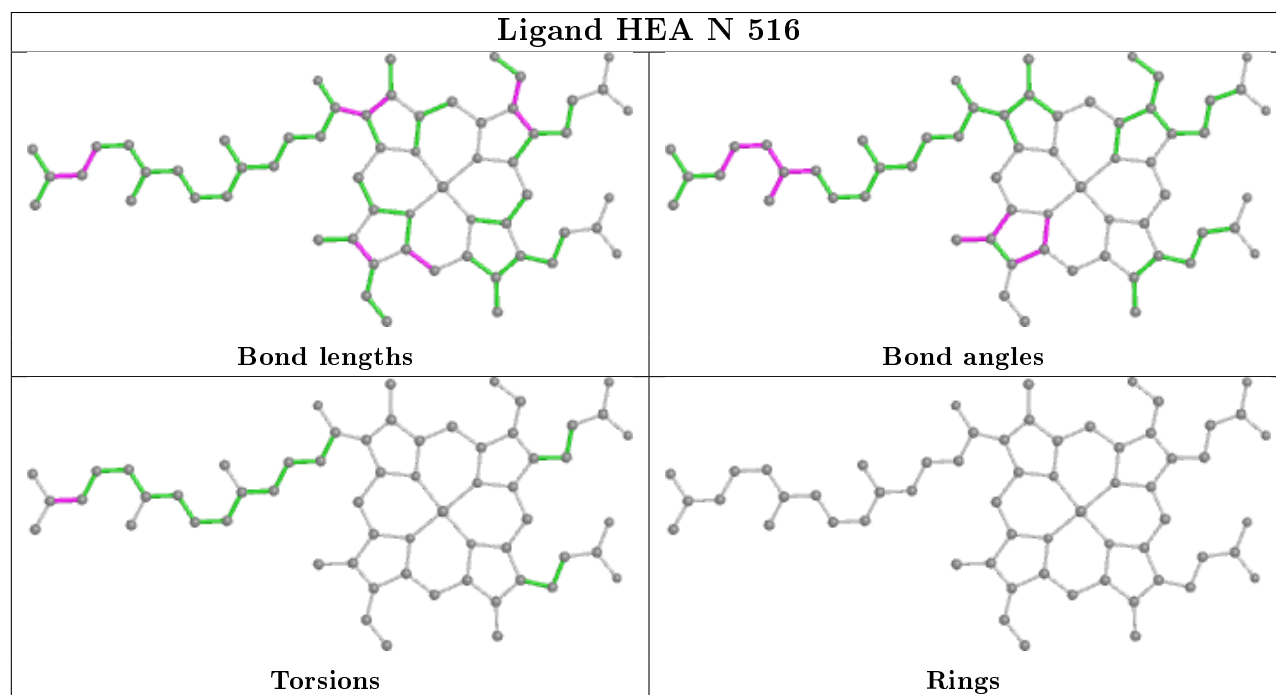
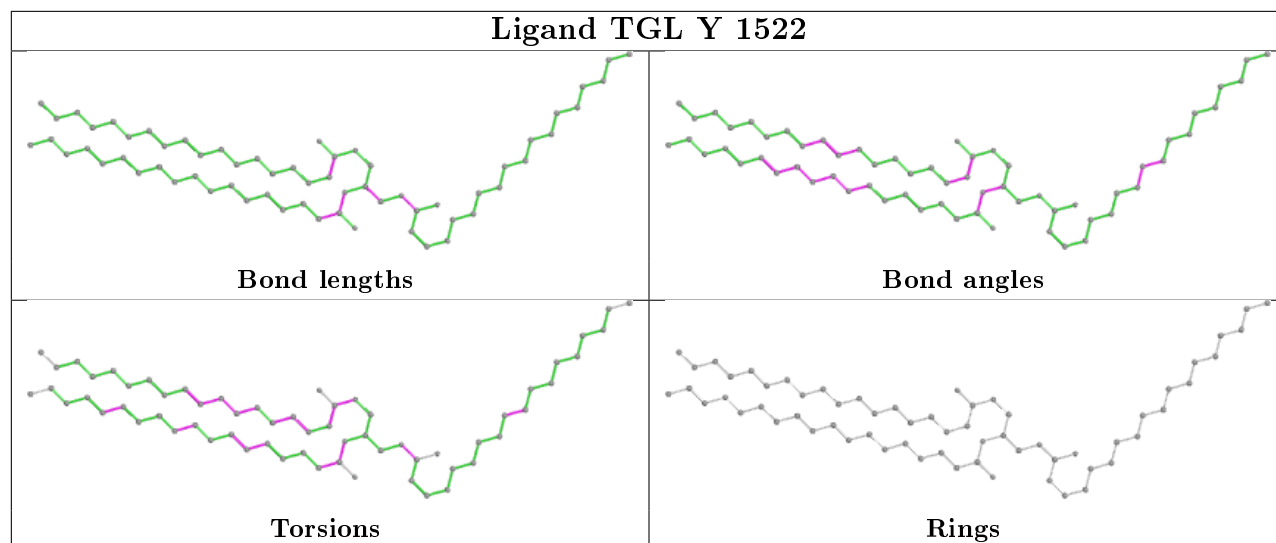
Ligand PGV N 1266



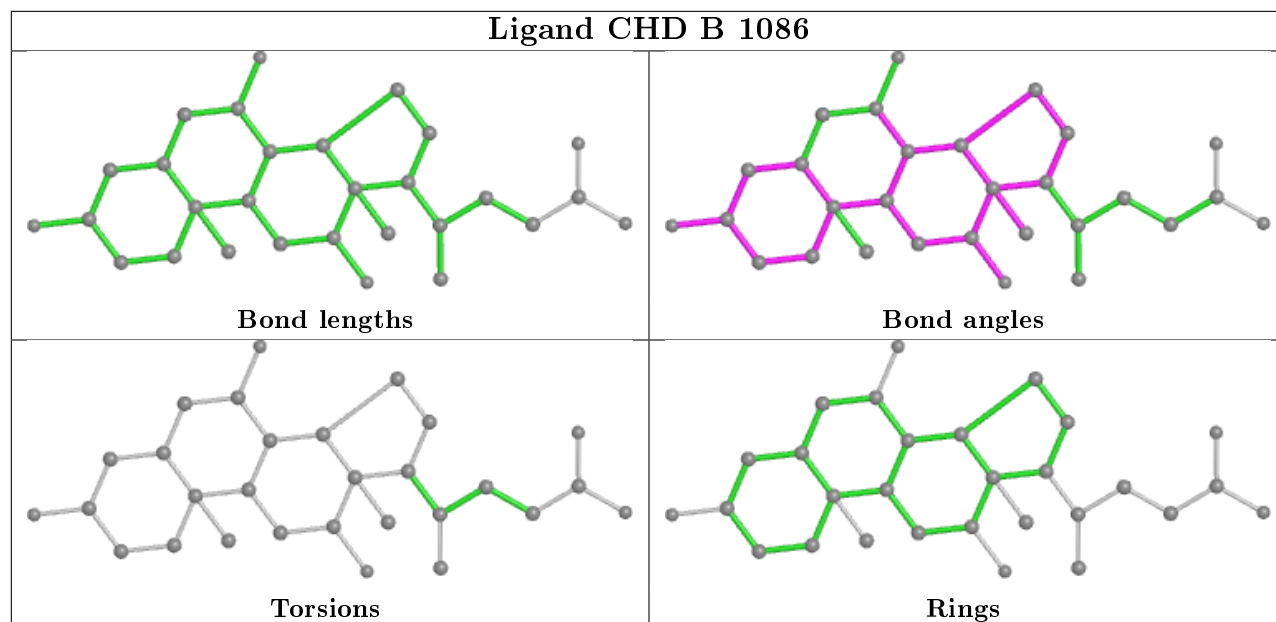
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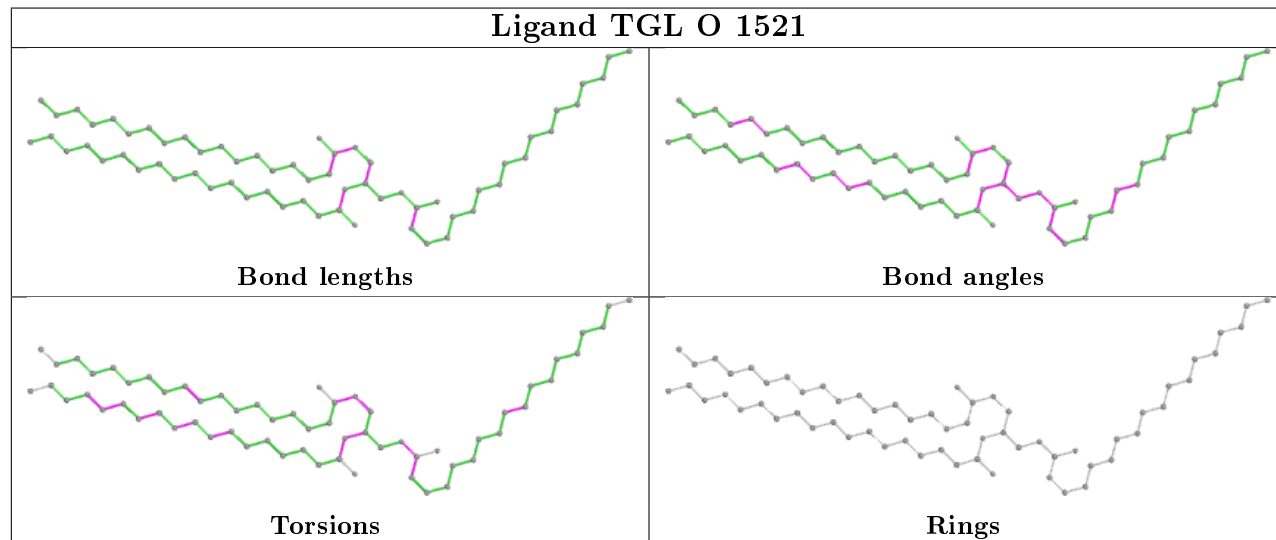




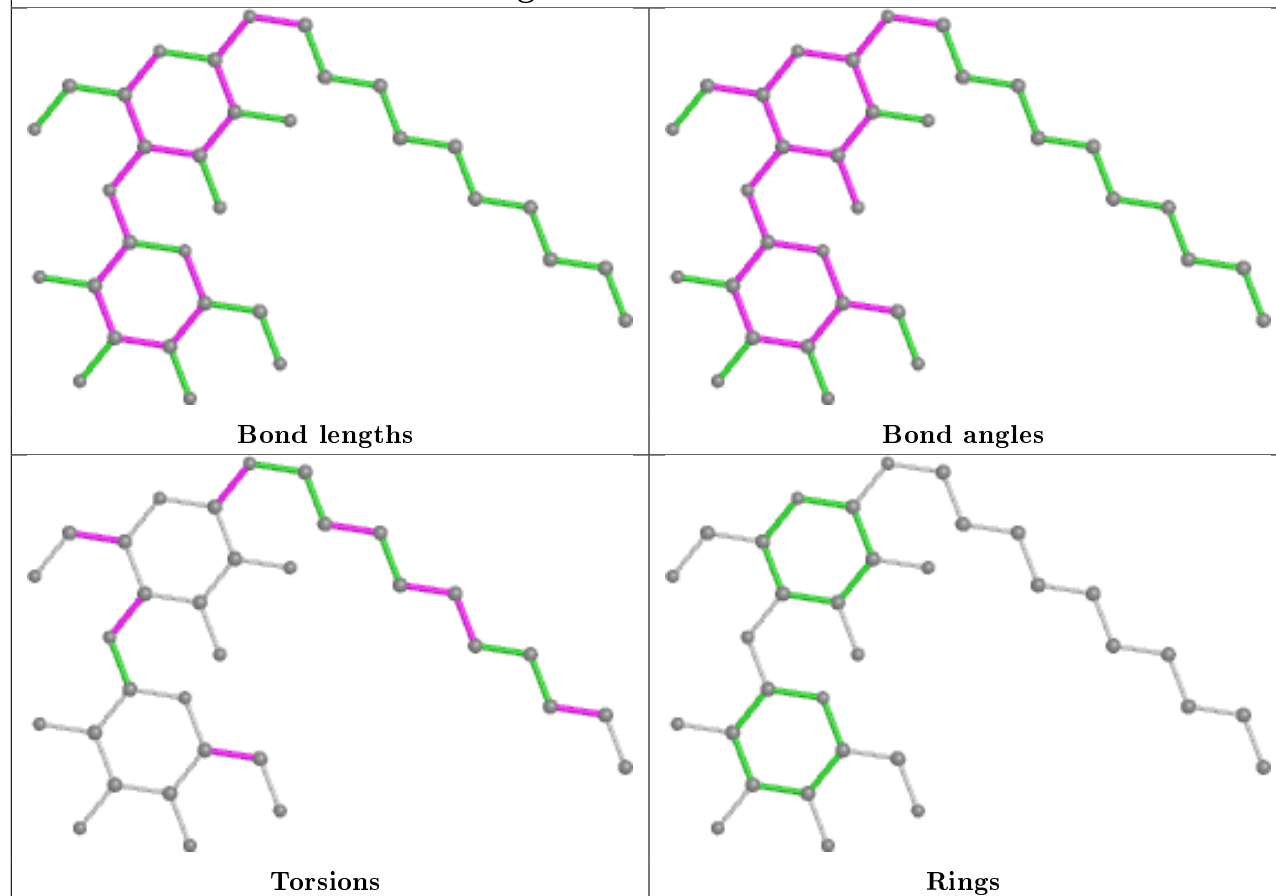
Ligand CHD B 1086



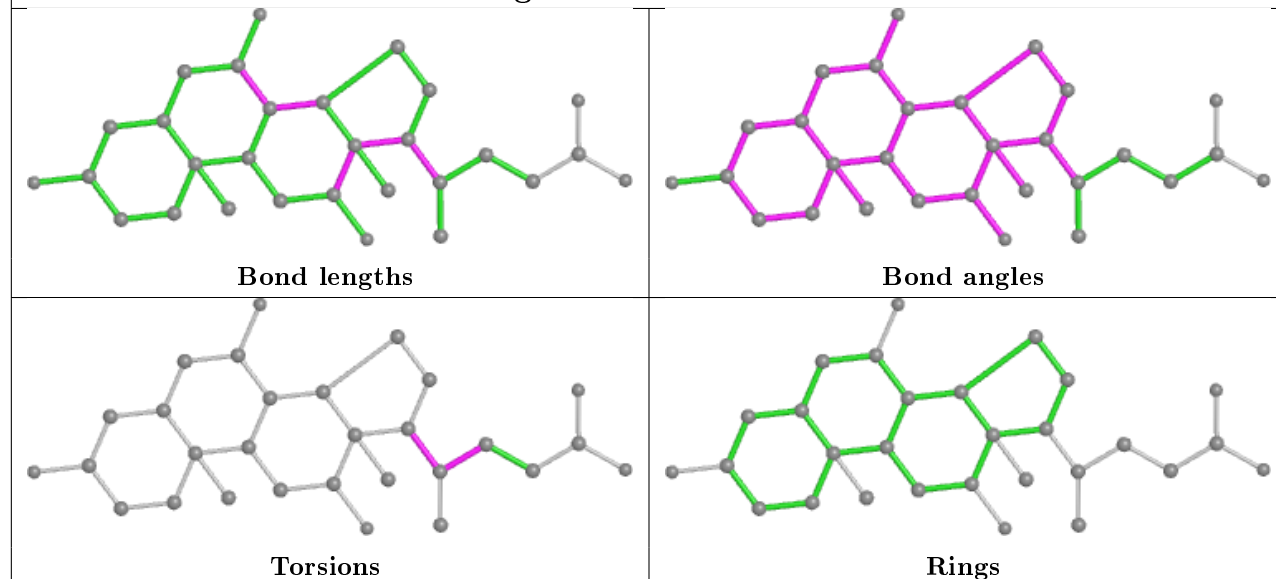
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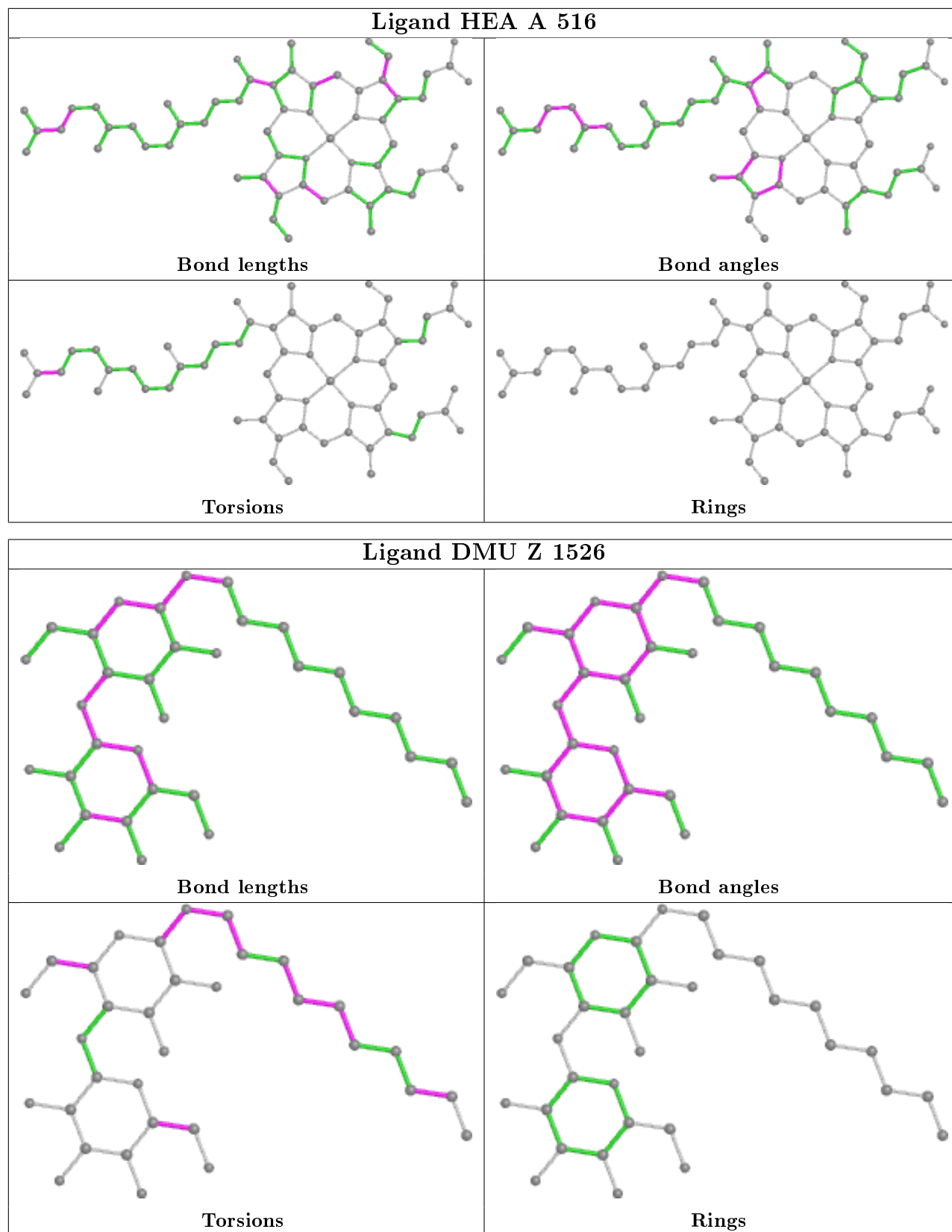


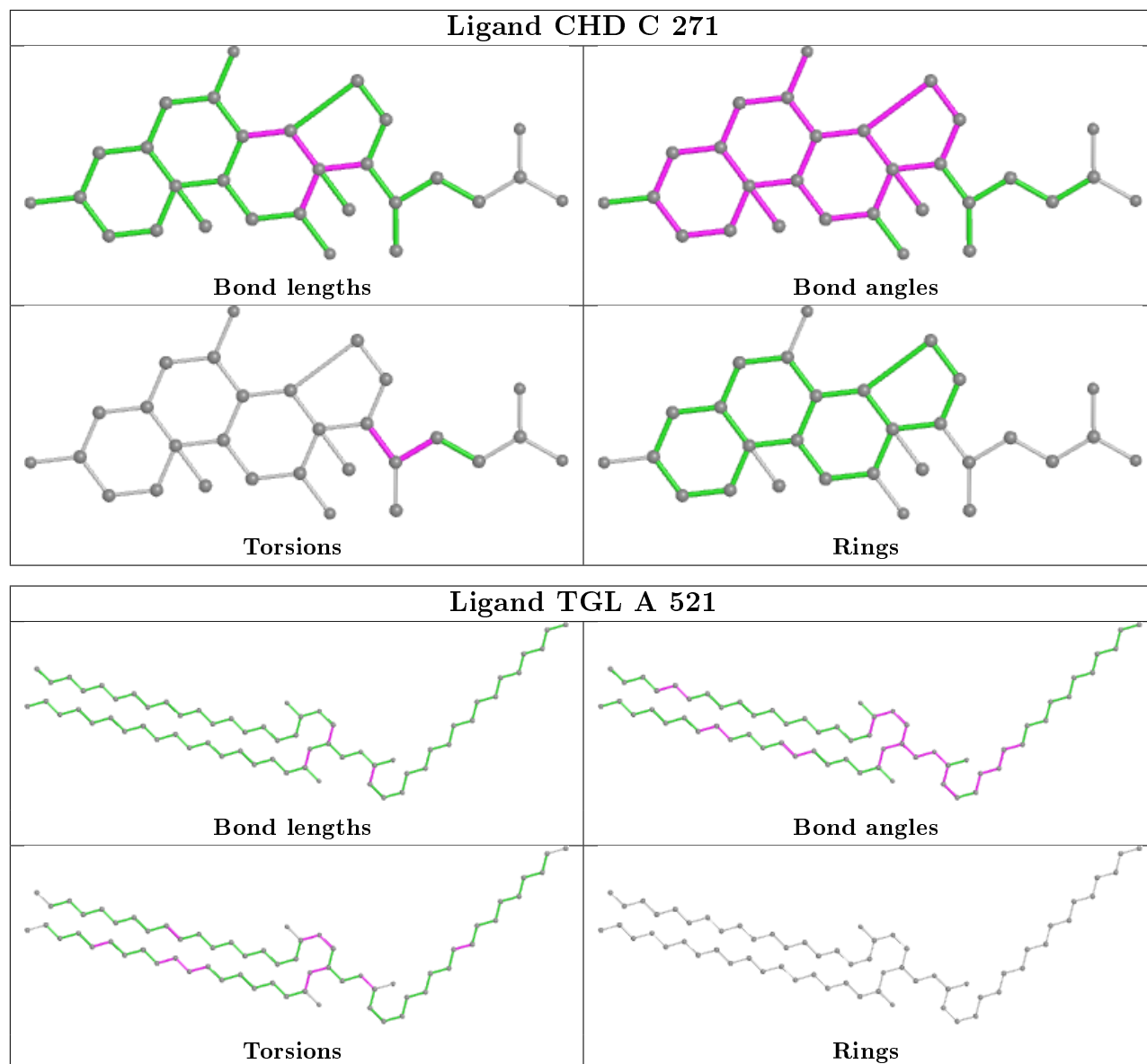
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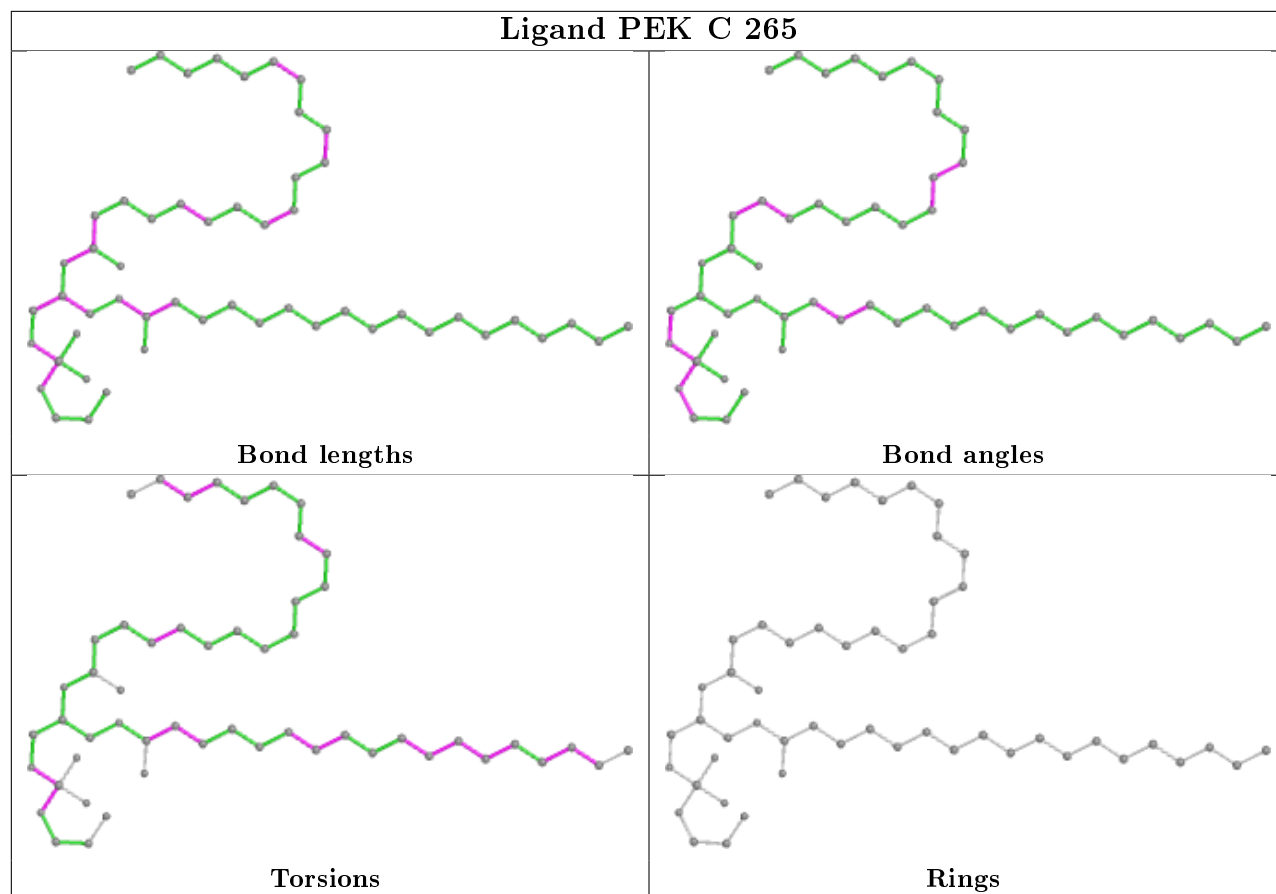


Ligand CHD W 1060

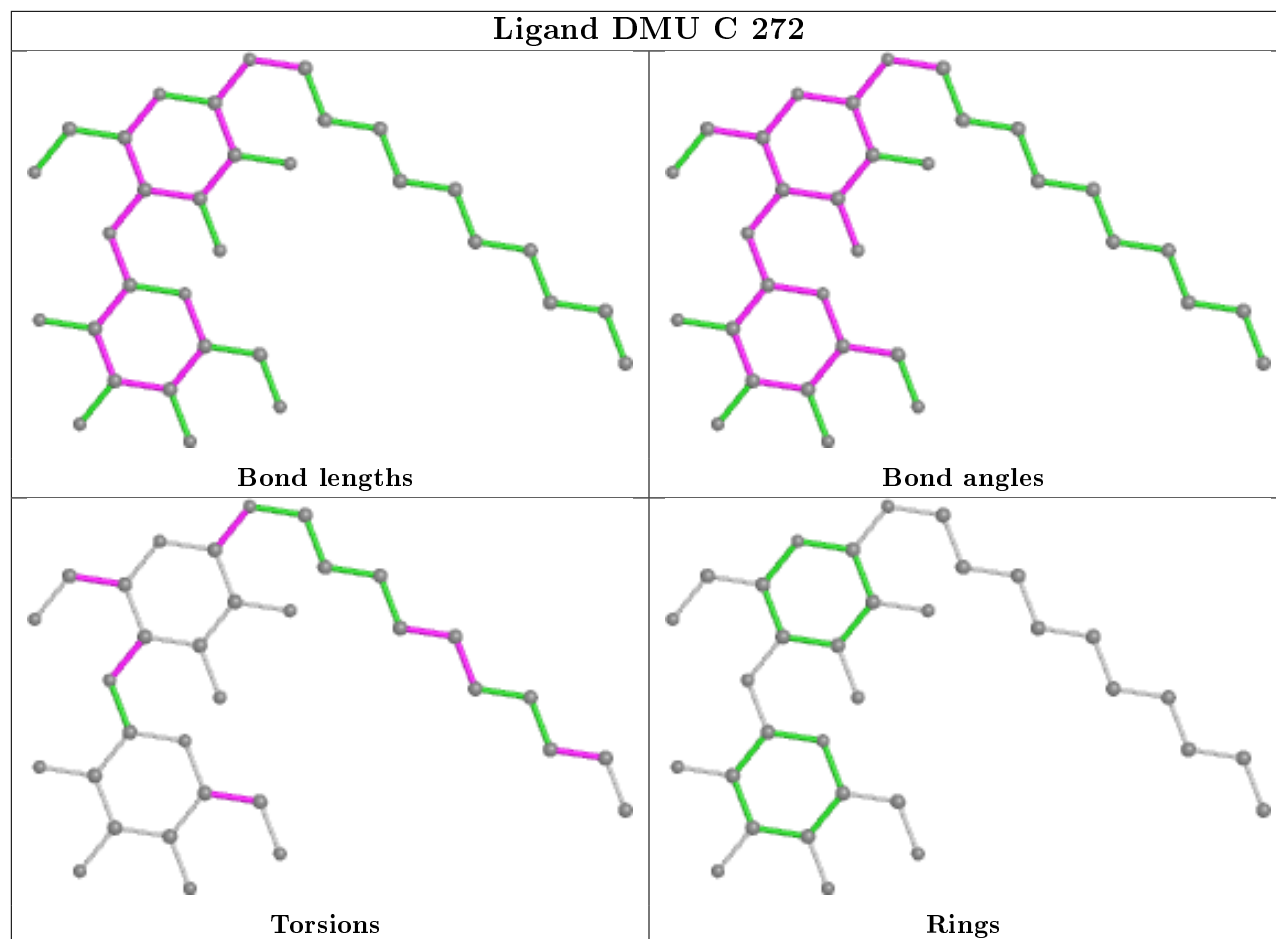




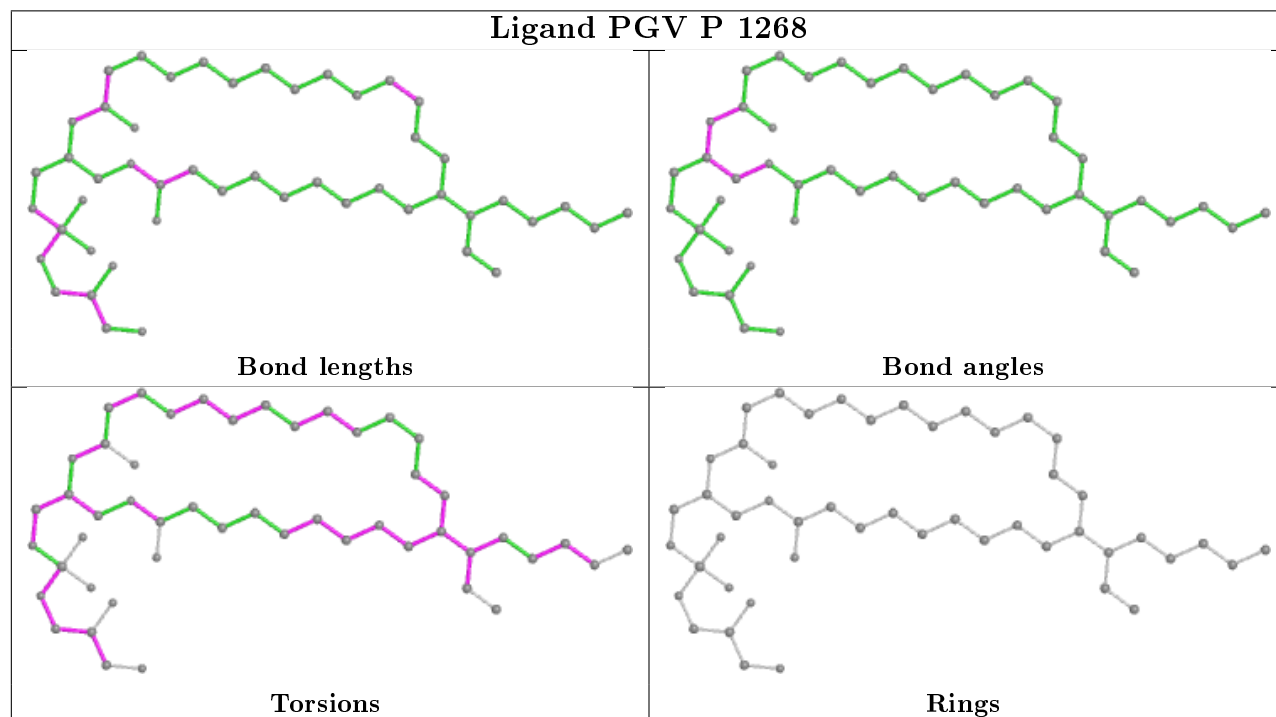


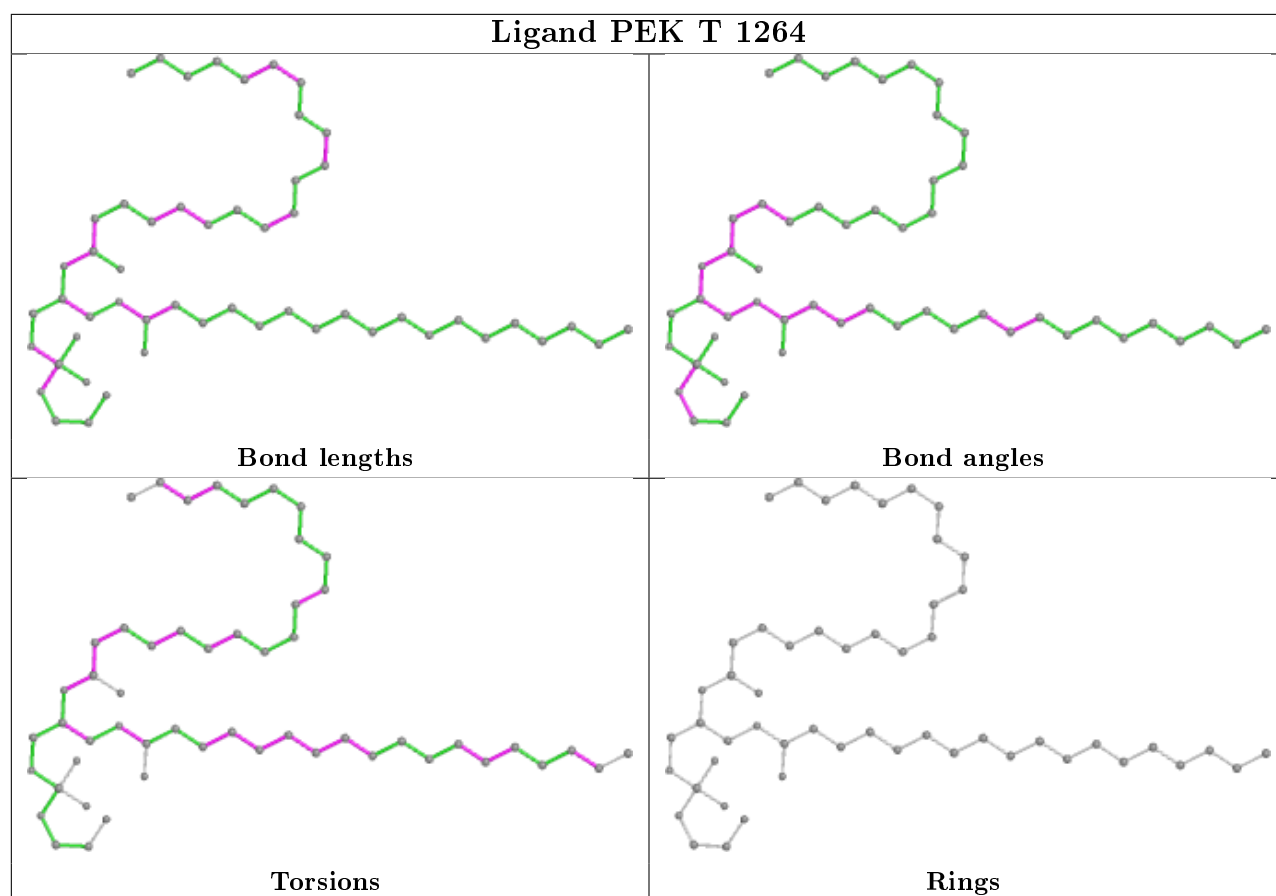
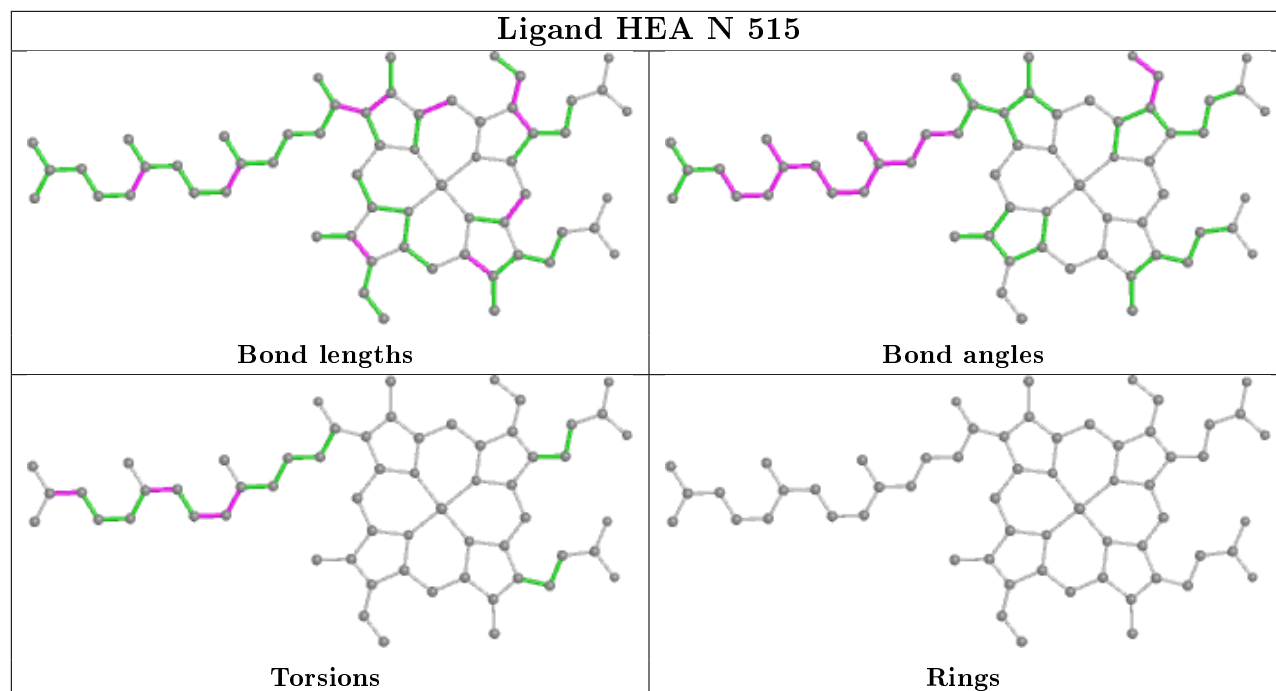


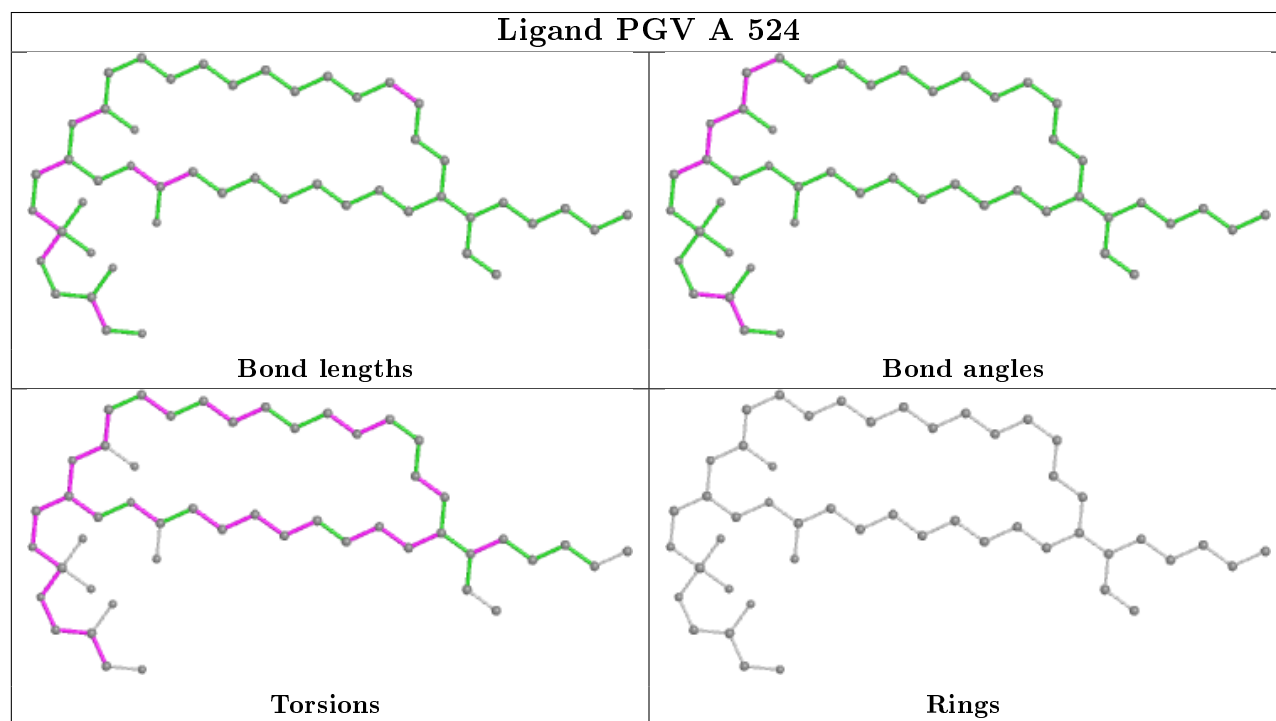
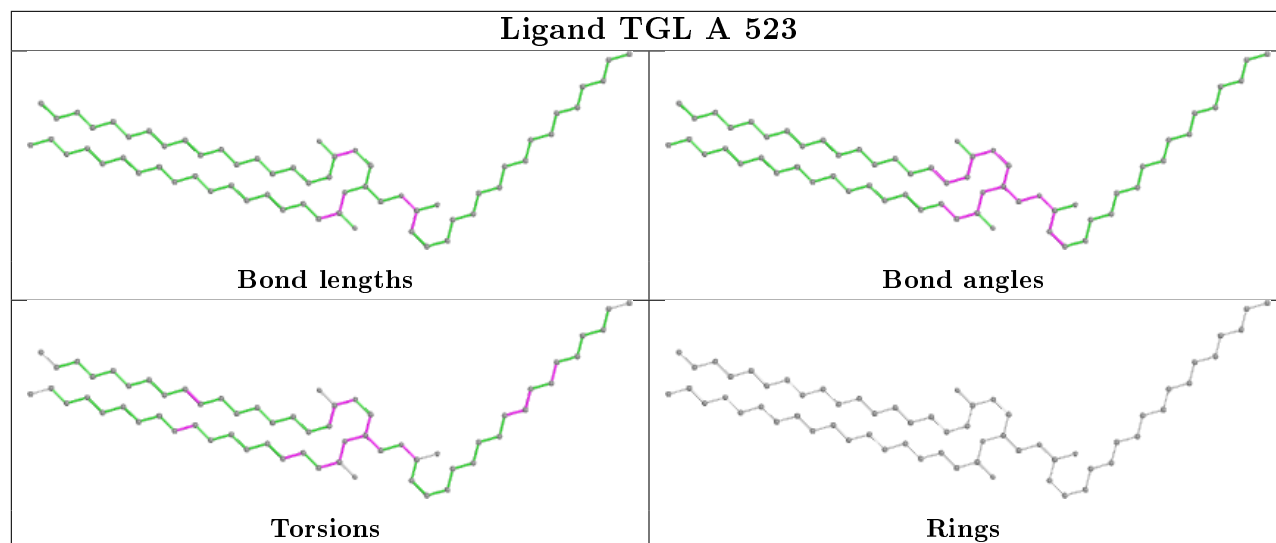
Ligand DMU C 272

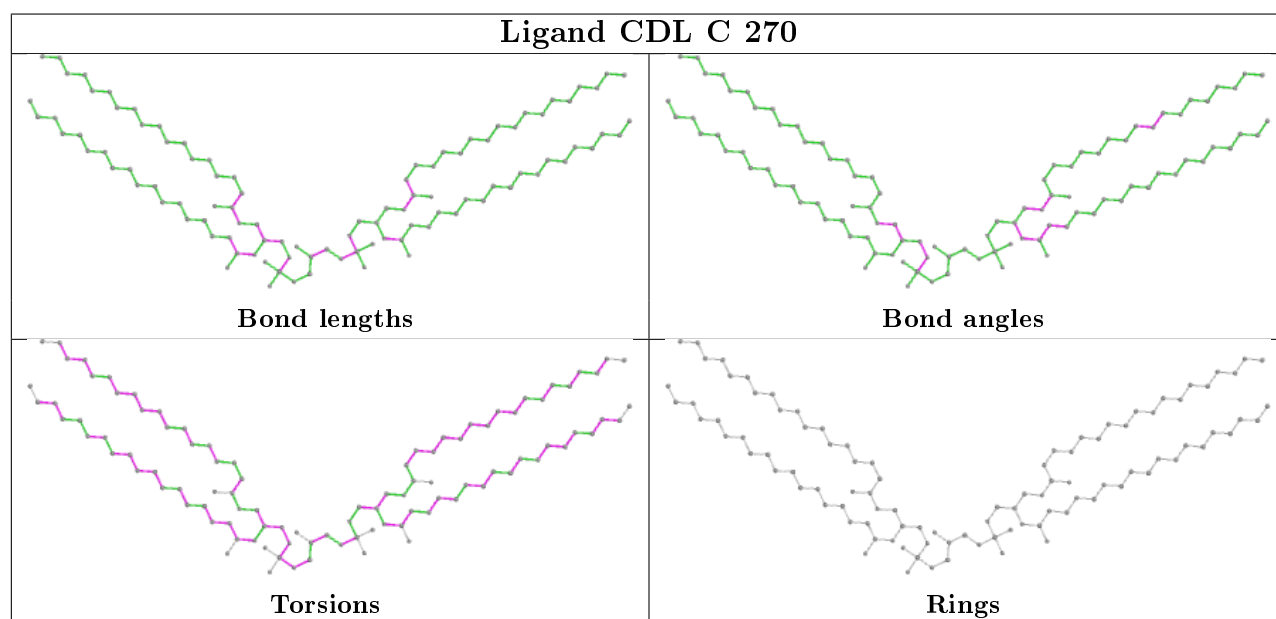
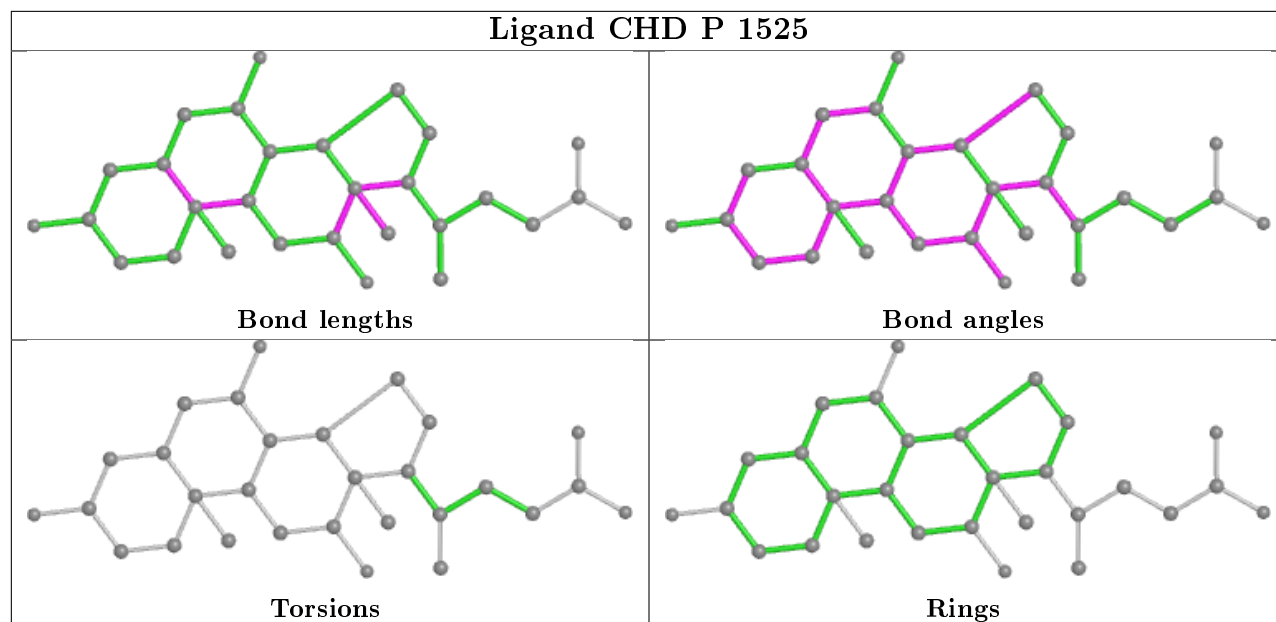


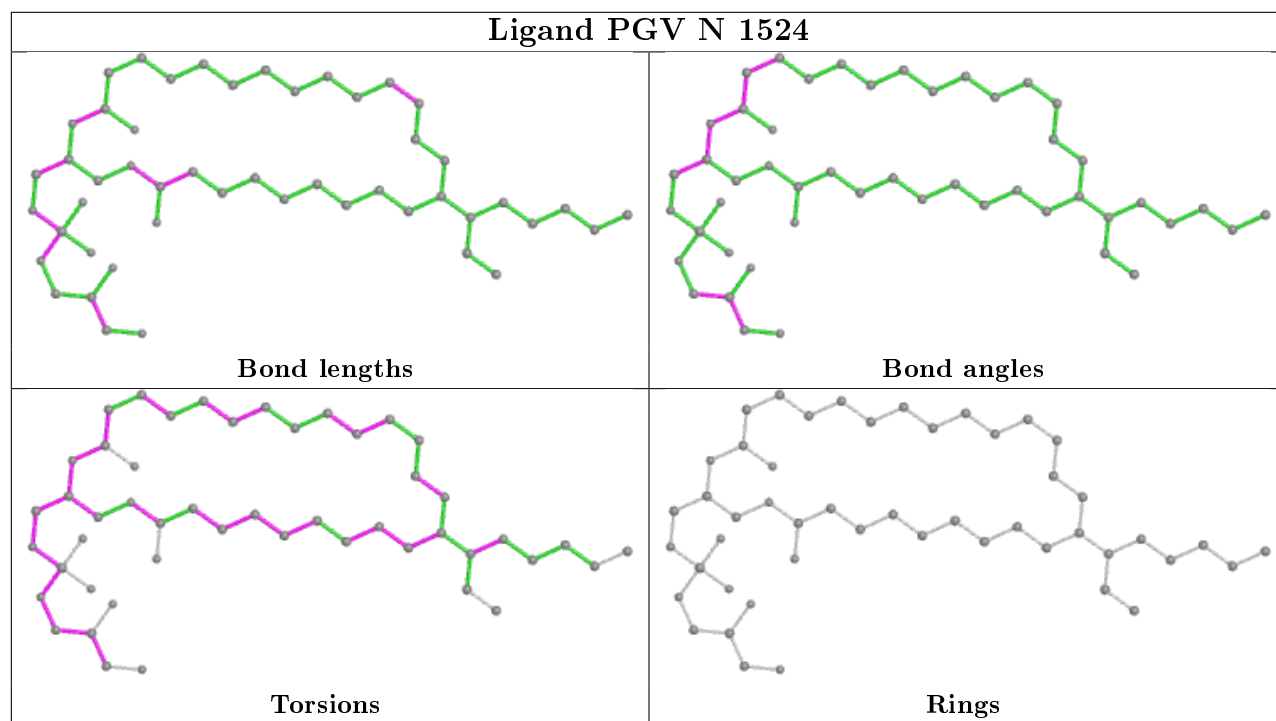
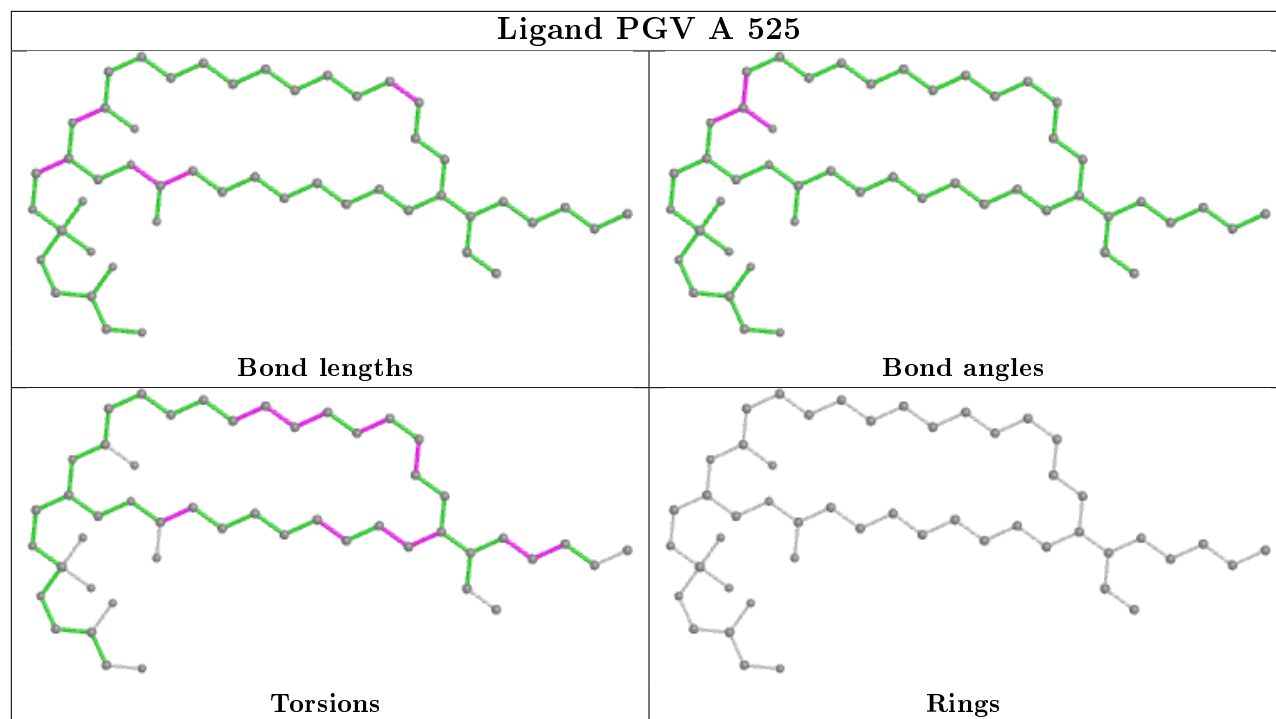
Ligand PGV P 1268

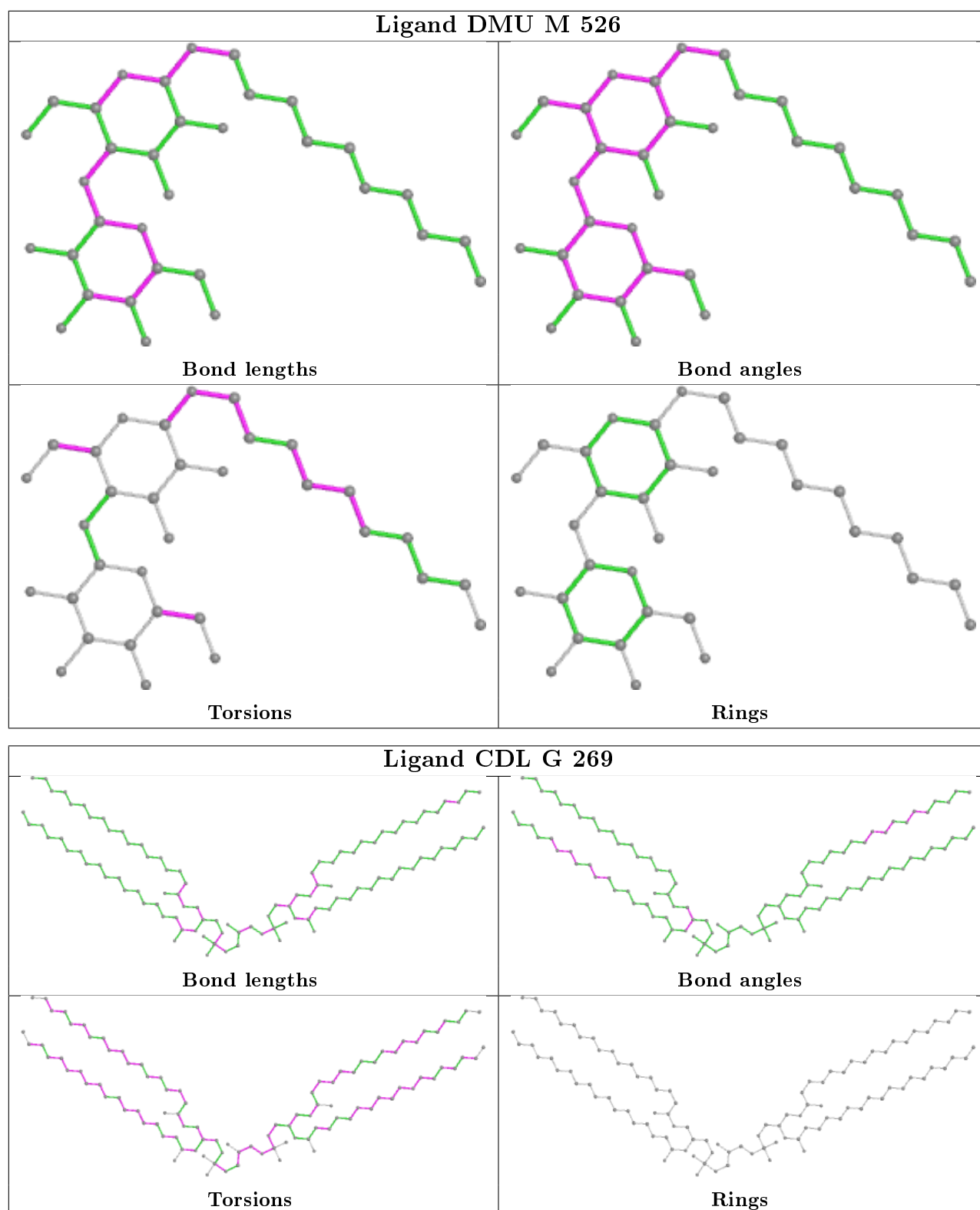












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.